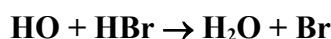


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iBrOx11

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

This data sheet updated: 30th January 2007.



$$\Delta H = -130.9 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(5.1 \pm 1.0) \times 10^{-12}$	295	Takacs and Glass, 1973	DF-EPR (a)
$(1.19 \pm 0.14) \times 10^{-11}$	249-416	Ravishankara et al., 1979	PLP-RF
$(6.01 \pm 0.32) \times 10^{-12}$	300	Husain et al., 1981	FP-RF
$(9.2 \pm 0.7) \times 10^{-12}$	~298	Jourdain et al., 1981	DF-EPR
$(1.12 \pm 0.045) \times 10^{-11}$	298 ± 4	Cannon et al., 1984	FP-LIF
$(1.1 \pm 0.1) \times 10^{-11}$	298	Ravishankara et al., 1985	PLP-RF/LIF
$(2.97 \pm 0.46) \times 10^{-11}$	170	Sims et al., 1994	PLP-LIF (b,c)
$(1.16 \pm 0.04) \times 10^{-11}$	295		
$(8 \pm 1) \times 10^{-12}$	173	Atkinson et al., 1997	FP-LIF (b,d)
$(1.5 \pm 0.4) \times 10^{-11}$	194		
$(1.0 \pm 0.3) \times 10^{-11}$	194		
$(1.3 \pm 0.2) \times 10^{-11}$	222		
$(1.1 \pm 0.1) \times 10^{-11}$	242		
$5.5 \times 10^{-12} \exp[(204 \pm 45)/T]$	230-360	Bedjanian et al., 1999	DF-MS (e)
$(1.11 \pm 0.12) \times 10^{-11}$	298		
$(9.36 \pm 2.74) \times 10^{-12}$	185	Jaramillo and Smith, 2001;	FP-LIF (b,f,g)
$(1.01 \pm 0.15) \times 10^{-11}$	224	Jaramillo et al., 2002	

Comments

- Rate coefficient obtained from a computer simulation of 4 reactions.
- Expansion of gas through a Laval nozzle to provide a collimated flow of cold gas at a uniform temperature, density and velocity.
- Experiments were carried out over the temperature range 23-295 K, with the measured rate coefficient decreasing with increasing temperature from $(1.07 \pm 0.04) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 23 K to $(1.16 \pm 0.04) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K. Combined with the rate coefficients of Ravishankara et al. (1979), the temperature-dependent expression $k = (1.26 \pm 0.24) \times 10^{-11} (T/298)^{-0.86 \pm 0.10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ was derived.
- Rate coefficients were measured over the temperature range 76-242 K, with the rate coefficient decreasing from $(3.0 \pm 0.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 92 K and $(2.9 \pm 0.9) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 76 K to $(1.1 \pm 0.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 242 K. Above 150 K the rate coefficient was independent of temperature, within the experimental uncertainties.
- The cited Arrhenius expression is obtained from a unit-weighted least-squares analysis of the measured rate coefficients. The cited uncertainty is one least-squares standard deviation.

- (f) Rate coefficients were obtained over the temperature range 120-224 K for HO + HBr, DO + HBr, HO + DBr and DO + DBr (Jaramillo and Smith, 2001), and over the temperature range 48-224 K for HO + HBr (Jaramillo et al., 2002).
- (g) The rate coefficients reported by Jaramillo and Smith (2001) have been re-evaluated by Mullen and Smith (2005), and the revised values are cited in the table. Mullen and Smith (2005) measured rate coefficients for HO + HBr (and HO + DBr, DO + HBr and DO + DBr) at 53, 83 and 135 K using a pulsed Laval nozzle with LIF detection of HO and DO radicals. A fit of the data of Ravishankara et al. (1979), Sims et al. (1994), Atkinson et al. (1997), Bedjanian et al. (1999), Jaramillo and Smith (2001) [using the rate coefficients as re-evaluated by Mullen and Smith (2005)], Jaramillo et al. (2002) [rate coefficients at 48 and 97 K] and Mullen and Smith (2005) for HO + HBr resulted in $k = 1.06 \times 10^{-11} (T/298)^{-(0.90 \pm 0.11)}$ cm³ molecule⁻¹ s⁻¹ over the temperature range 23-360 K.

Preferred Values

$k = 6.7 \times 10^{-12} \exp(155/T)$ cm³ molecule⁻¹ s⁻¹ over the temperature range 180-370 K.

$k = 1.1 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K.

Reliability

$\Delta \log k = \pm 0.10$ at 298 K.

$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The studies of Sims et al. (1994), Atkinson et al. (1997), Jaramillo and Smith (2001), Jaramillo et al. (2002) and Mullen and Smith (2005), carried out using expansions through a Laval nozzle to achieve temperatures down to 23 K, show reaction rate coefficients which increase with decreasing temperature, as does the 230-360 K study of Bedjanian et al. (1999). There is, however, a significant amount of scatter in the low temperature (<250 K) rate coefficients obtained by Sims et al. (1994), Atkinson et al. (1997), Jaramillo and Smith (2001) [as revised by Mullen and Smith, 2005], Jaramillo et al. (2002) and Mullen and Smith (2005). The preferred values are obtained from a least-squares analysis of the 230-369 K rate coefficients of Ravishankara et al. (1979), Ravishankara et al. (1985) and Bedjanian et al. (1999). The preferred values are in good agreement with the room temperature rate coefficients of Jourdain et al. (1981) and Cannon et al. (1984), and are consistent with the <250 K rate data of Sims et al. (1994), Atkinson et al. (1997), Jaramillo and Smith (2001), Jaramillo et al. (2002) and Mullen and Smith (2005). Accordingly, the preferred rate expression is judged to be applicable down to ~180 K.

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- Expression of Mullen and Smith (2005)
- Recommendation (180-370 K)
- Ravishankara et al. (1979)
- △ Ravishankara et al. (1985)
- Sims et al. (1994)
- ▲ Atkinson et al. (1997)
- Bedjanian et al. (1999)
- ▽ Jaramillo and Smith (2001)
- ▲ Jaramillo et al. (2002)
- ◆ Mullen and Smith (2005)

