# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oBrOx18; VII.A3.3

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## $HO + CH_2BrCH_2Br \rightarrow CHBrCH_2Br + H_2O$

### Rate coefficient data (*k*)

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | $T$/K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $(2.50 \pm 0.55) \times 10^{-13}$ | 296 | Howard and Evenson (1976) | DF-LMR (a) |
| $(1.46\pm0.26) \times 10^{-11}$ exp[-(1283±136)/T)] | 294-365 | Qiu et al. (1992) | DF-RF (b) |
| $1.86 \times 10^{-13}$ | 294 | | |
| *Relative Rate Coefficients* | | | |
| $(2.15 \pm 0.45) \times 10^{-13}$ | 300 | Arnts et al. (1989) | RR (c) |

### Comments

(a) HO radicals were generated by the reaction of H atoms with $NO_2$ in 0.1-1.0 kPa (1-10 mbar) of helium diluent.

(b) HO radicals were produced by the reaction of F atoms with $H_2O$ in 2-3 Torr (2.7-4.0 mbar) of argon diluent gas. The value given at 298 K above is the average of the measurements reported by Qiu et al. (1992) at this temperature.

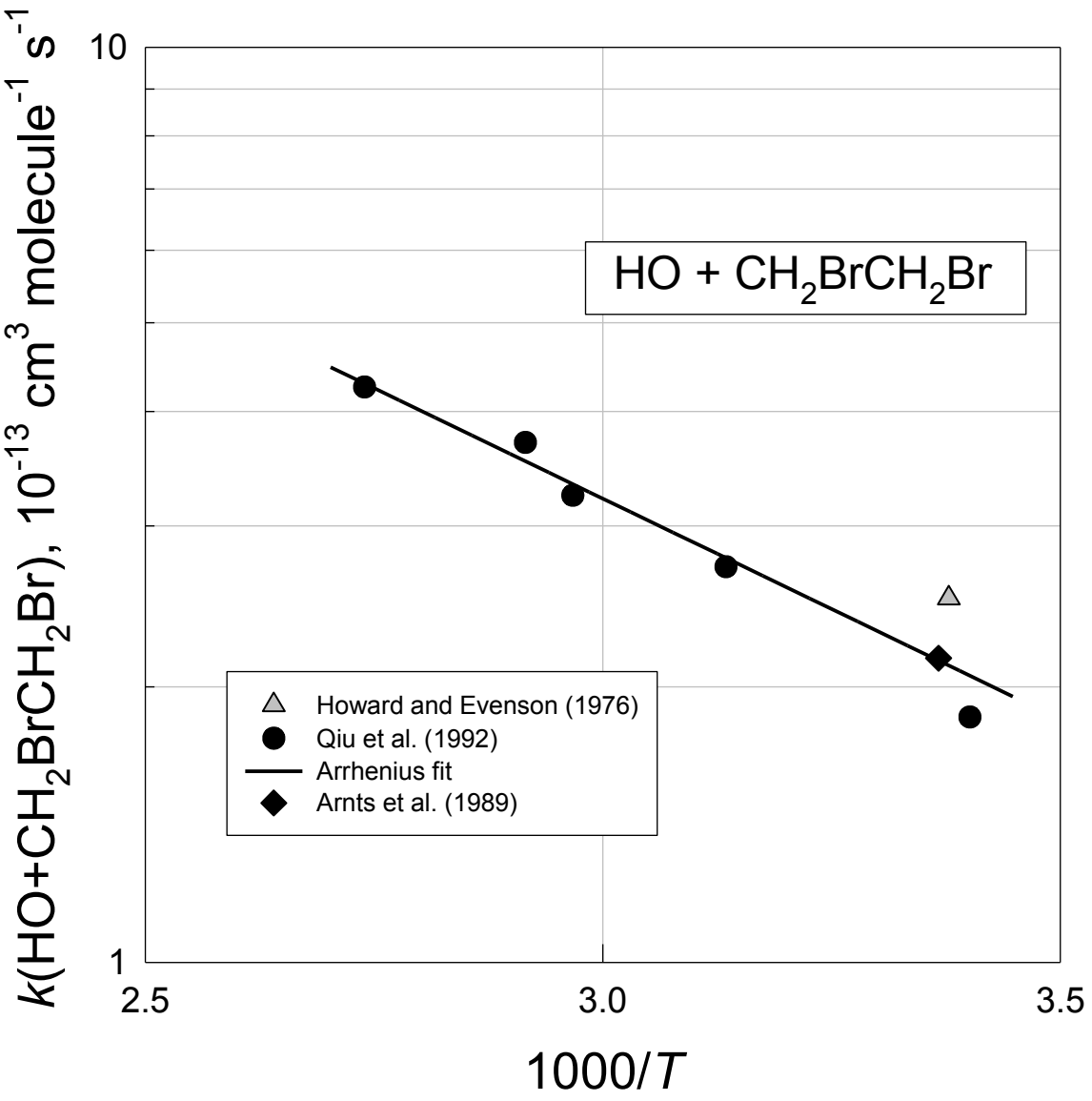
(c) The rate coefficient ratio $k(HO+CH_2BrCH_2Br)/k(HO+C_2H_6) = 0.88 \pm 0.18$ was placed on an absolute basis using $k(HO+C_2H_6) = 1.49 \times 10^{-17}\ T^2 \exp(-499/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson et al., 2006).

### Preferred Values

| Parameter | Value | $T$/K |
|---|---|---|
| $k$ /cm$^3$ molecule$^{-1}$ s$^{-1}$ | $2.22 \times 10^{-13}$ | 298 |
| $k$ /cm$^3$ molecule$^{-1}$ s$^{-1}$ | $7.69 \times 10^{-12}$ exp(-1056/T) | 290-370 |
| *Reliability* | | |
| $\Delta \log k$ | 0.1 | 298 |
| $\Delta$ E/R | ± 300 | |

*Comments on Preferred Values*

The absolute rate coefficients of Howard and Evenson (1976), Qiu et al. (1992) and Arnts et al. (1989) are in reasonable agreement at ambient temperature. Fitting the Arrhenius expression to the combined data set from the three studies gives $k = 7.69 \times 10^{-12}$ exp(-1056/T) cm$^3$ molecule$^{-1}$ s$^{-1}$ (Calvert et al., 2010) which is recommended over the range 290-370 K.

### References

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