# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx29


This data sheet updated: 15th March 2006.

$$HO + CHF_2CHO \rightarrow H_2O + CHF_2CO \quad (1)$$
$$\rightarrow H_2O + CF_2CHO \quad (2)$$

$\Delta H°(1) = -110.4$ kJ mol$^{-1}$

## Rate coefficient data ($k = k_1 + k_2$)

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $(1.7 \pm 0.2) \times 10^{-12}$ | 298 ± 2 | Scollard et al., 1993 | PLP-RF |
| *Relative Rate Coefficients* | | | |
| $(1.3 \pm 0.3) \times 10^{-12}$ | 298 ± 2 | Scollard et al., 1993 | RR (a) |
| $(1.8 \pm 0.4) \times 10^{-12}$ | 298 ± 2 | Sellevåg et al., 2005 | RR (b) |

## Comments

(a) HO radicals were generated by the photolysis of $CH_3ONO$ (or $C_2H_5ONO$)-NO-$CHF_2CHO$-toluene-air mixtures at 1 bar pressure. The concentrations of $CHF_2CHO$ and toluene were measured by GC and FTIR spectroscopy. The measured rate coefficient ratio of $k$(HO + $CHF_2CHO$)/$k$(HO + toluene) is placed on an absolute basis by using a rate coefficient of $k$(HO + toluene) = $5.63 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Calvert et al., 2002).

(b) HO radicals were generated by the photolysis of $O_3$ in the presence of $H_2$-$CHF_2CHO$-propane-air mixtures at 1 bar pressure. The concentrations of $CHF_2CHO$ and propane were measured by FTIR spectroscopy. The measured rate coefficient ratio of $k$(HO + $CHF_2CHO$)/$k$(HO + $C_3H_8$) = 1.62 ± 0.04 is placed on an absolute basis by using a rate coefficient of $k$(HO + $C_3H_8$) = $1.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (IUPAC, 2006)

## Preferred Values

$k = 1.6 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.

*Reliability*

$\Delta \log k = \pm 0.2$ at 298 K.

*Comments on Preferred Values*

The absolute and relative rate coefficients of Scollard et al. (1993) and Sellevåg et al. (2005) are in good agreement, and the preferred value is the average of these rate coefficients. The reaction is expected to proceed by pathway (1) (Scollard et al., 1993), which is supported by the quantum chemical calculations of and Sellevåg et al. (2005).

## References

Calvert, J. G., Atkinson, R., Becker, K. H., Kamens, R. M., Seinfeld, J. H., Wallington, T. J. and Yarwood, G.: The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons, Oxford

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Scollard, D. J., Treacy, J. J., Sidebottom, H. W., Balestra-Garcia, C., Laverdet, G., Le Bras, G., MacLeod, H. and Téton, S.: J. Phys. Chem. 97, 4683, 1993.
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