

## IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet X\_VOC26

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### Cl + CH<sub>3</sub>C(O)OONO<sub>2</sub> → products

#### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(3.7 \pm 1.7) \times 10^{-13}$	298	Tsalkani <i>et al.</i> , 1988 <sup>1</sup>	DF-EPR
<i>Relative Rate Coefficients</i>			
$< 7 \times 10^{-15}$	295 ± 2	Wallington <i>et al.</i> , 1990 <sup>2</sup>	RR (a)

#### Comments

- (a) Cl atoms were generated by the photolysis of Cl<sub>2</sub> in Cl<sub>2</sub>-air-CH<sub>3</sub>C(O)OONO<sub>2</sub>-CH<sub>4</sub> mixtures at 930 mbar (700 Torr) total pressure, with the CH<sub>3</sub>C(O)OONO<sub>2</sub> and CH<sub>4</sub> concentrations being monitored by FTIR absorption spectroscopy. Upper limit to relative rate coefficient ratio placed on an absolute basis by use of  $k(\text{Cl} + \text{CH}_4) = 9.9 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .<sup>3</sup>

#### Preferred Values

$$k < 2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

#### Comments on Preferred Values

The preferred value is based on the relative rate coefficient measurement of Wallington *et al.*,<sup>2</sup> in which no reaction of CH<sub>3</sub>C(O)OONO<sub>2</sub> was observed in the presence of Cl atoms. In both the relative rate study of Wallington *et al.*<sup>2</sup> and the absolute rate study of Tsalkani *et al.*,<sup>1</sup> the major impurity in the CH<sub>3</sub>C(O)OONO<sub>2</sub> samples would be the C<sub>12</sub> or C<sub>13</sub> alkane solvent, respectively. While this was of no consequence in the relative rate study of Wallington *et al.*,<sup>2</sup> the presence of ~0.1% tridecane in the CH<sub>3</sub>C(O)OONO<sub>2</sub> sample used by Tsalkani *et al.*<sup>1</sup> could account for the Cl reaction rate observed; their CH<sub>3</sub>C(O)OONO<sub>2</sub> sample was >99% pure from IR measurements. The upper limit cited here is a factor of ~3 higher than measured by Wallington *et al.*<sup>2</sup> to allow for greater uncertainties.

#### References

- <sup>1</sup> N. Tsalkani, A. Mellouki, G. Poulet, G. Toupance, and G. Le Bras, *J. Atmos. Chem.* **7**, 409 (1988).
- <sup>2</sup> T. J. Wallington, J. M. Andino, J. C. Ball, and S. M. Japar, *J. Atmos. Chem.* **10**, 301 (1990).
- <sup>3</sup> IUPAC (2002), <http://www.iupac-kinetic.ch.cam.ac.uk/>