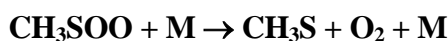


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SO<sub>x</sub>57

Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys. 4, 1461, 2004; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, (<http://iupac.pole-ether.fr>).

This data sheet last evaluated: November 2017; last change in preferred values: November 2001.



$$\Delta H^\circ = 48.9 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data

| $k/\text{s}^{-1}$                           | Temp./K | Reference               | Technique/<br>Comments |
|---|---------|-------------------------|------------------------|
| <i>Absolute Rate Coefficients</i>           |         |                         |                        |
| $(1.99 \pm 0.74) \times 10^3$ 107 mbar (He) | 216     | Turnipseed et al., 1992 | (a)                    |
| $(3.20 \pm 0.80) \times 10^3$ 107 mbar (He) | 222     |                         |                        |
| $(9.1 \pm 2.6) \times 10^3$ 107 mbar (He)   | 233     |                         |                        |
| $(1.00 \pm 0.12) \times 10^4$ 107 mbar (He) | 237     |                         |                        |
| $(1.28 \pm 0.12) \times 10^4$ 107 mbar (He) | 242     |                         |                        |
| $(2.4 \pm 0.4) \times 10^4$ 107 mbar (He)   | 250     |                         |                        |
| $>3.5 \times 10^4$ 107 mbar (He)            | 258     |                         |                        |

### Comments

- (a) Pulsed laser photolysis system with LIF detection of CH<sub>3</sub>S radicals. The formation and decay rate coefficients of CH<sub>3</sub>SOO radicals were derived from the observed time-concentration profiles of CH<sub>3</sub>S radicals in the presence of O<sub>2</sub>. The measured rate coefficients for the reactions CH<sub>3</sub>S + O<sub>2</sub> → CH<sub>3</sub>SOO were observed to vary with total pressure and with the diluent gas.
- (b) See Comments on Preferred Values.

### Preferred Values

The preferred data are from Turnipseed et al. (1992). These data at 107 mbar He are described by  $k(210\text{-}250 \text{ K}) = 3.5 \times 10^{10} \exp(-3560/T) \text{ s}^{-1}$ .

### *Reliability*

$\Delta \log k = \pm 0.3$  at 107 mbar He over the temperature range 216-250 K.

### *Comments on Preferred Values*

The data presented by Turnipseed et al. (1992) were the first reported for the dissociation of the CH<sub>3</sub>SOO radical (see also the data sheet in this evaluation for the reverse reaction CH<sub>3</sub>S + O<sub>2</sub> + M → CH<sub>3</sub>SOO + M). In the atmosphere, ~33% of CH<sub>3</sub>S radicals will be present as the CH<sub>3</sub>SOO adduct at 298 K and ground level, with the [CH<sub>3</sub>SOO]/[CH<sub>3</sub>S] ratio being strongly temperature dependent. Measurements of the equilibrium constant for formation and dissociation of CH<sub>3</sub>SOO from 216 to 258 K by Turnipseed et al. (1992) were consistent with results from Butkovskaya and Barnes (2002) as analysed by Chu and Lee (2010) (see the discussion in Burkholder et al., 2015).

### **References**

- Burkholder, J. B., Sander, S. P., Abbatt, J., Barker, J. R., Huie, R. E., Kolb, C. E., Kurylo, M. J., Orkin, V. L., Wilmouth, D. M., and Wine, P. H.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, NASA Panel for Data Evaluation, Evaluation Number 18, JPL Publication 15-10, 2015.
- Butkovskaya, N. I., and Barnes, I.: NATO Science Series 16, 147, 2002.
- Chu, L.-K., and Lee, Y.-P.: J. Chem. Phys. 133, 184303, 2010.
- Turnipseed, A. A., Barone, S. B., and Ravishankara, A. R.: J. Phys. Chem. 96, 7502, 1992.