

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet CGI\_28

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### (CH<sub>3</sub>)<sub>2</sub>COO + HC(O)OH → products

#### Rate coefficient data

<i>k</i> /cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Temp./K	Reference	Technique/Comments
<i>Absolute Rate Coefficients</i> (3.1 ± 0.2) × 10 <sup>-10</sup>	293	Chhantyal-Pun et al., 2018	PLP-CRDS (a)

#### Comments

- (a) (CH<sub>3</sub>)<sub>2</sub>COO was produced by 355 nm laser photolysis of 2,2-diiodopropane in the presence of HC(O)OH, O<sub>2</sub> and N<sub>2</sub> at a total pressure of 13 mbar; and characterized by cavity ringdown ultraviolet absorption spectroscopy. Experiments were carried out under pseudo-first order conditions, with excess concentrations of HC(O)OH, and *k* was derived from the linear dependence of the decay constant on [HC(O)OH].

#### Preferred Values

Parameter	Value	T/K
<i>k</i> /cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	3.1 × 10 <sup>-10</sup>	298
<i>Reliability</i> Δ log <i>k</i>	± 0.1	298

#### Comments on Preferred Values

The preferred value of *k* at 298 K is based on the determination reported in the sole kinetics study of Chhantyal-Pun et al. (2018). The extremely rapid rates of the reactions of sCIs with organic acids have been interpreted using a dipole-capture model, with the results for a number of sCI-acid combinations being used to formulate a structure-activity relationship, SAR (Chhantyal-Pun et al., 2018). The temperature dependence in *k* is expected to be weak. Based on product measurements for the CH<sub>2</sub>OO + CF<sub>3</sub>C(O)OH reaction (using PIMS), the reactions are believed to proceed via an insertion reaction to form hydroperoxyl-esters, consistent with the results of theoretical studies (e.g. Aplincourt and Ruiz-Lopez, 2000).

## References

- Aplincourt, P. and Ruiz-Lopez, M. F.: J. Phys. Chem., A,104, 380, 2000.
- Chhantyal-Pun, R., Rotavera, B., McGillen, M. R., Khan, M. A. H., Eskola, A. J., Caravan, R. L., Blacker, L., Tew, D. P., Osborn, D. L., Percival, C. J., Shallcross, D. E. and Orr-Ewing A. J.: ACS Earth Space Chem., 2, 833, 2018.