

Task Group on Atmospheric Chemical Kinetic Data Evaluation– Data Sheet HO_x_VOC97

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HO + CH₃C(O)C(O)OH → products

Rate coefficient data (*k*)

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
4.9 × 10 ⁻¹⁴ exp [(276 ± 123)/T]	273-371	Mellouki and Mu, 2003	LP-LIF (a)
(1.2 ± 0.4) × 10 ⁻¹³	298		

Comments

- (a) Experiments conducted at 133 mbar He or N₂. HO was generated by the 355 nm photolysis of HONO and detected by LIF. Pyruvic acid was stored diluted in a glass bulb and its concentration calculated from its mixing ratio, partial flow rate and total pressure.

Preferred Values

Preferred Values

Parameter	Value	T/K
<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	1.2 × 10 ⁻¹³	298
	4.9 × 10 ⁻¹⁴ exp (280 /T]	260-380
<i>Reliability</i>		
Δ log <i>k</i>	± 0.2	298
Δ E/R	± 150	

Comments on Preferred Values

There is only one experimental study of the rate coefficient of this reaction (Mu and Mellouki, 2003). Considering the very limited database and the fact that the concentration of the excess reactant pyruvic acid, which has a high affinity for surfaces, was not measured in-situ we expand the error limits. There are no data on the products formed, though abstraction of an H-atom from the OH group is expected to be the dominant reaction pathway, resulting ultimately in formation of H₂O, CH₃CO and CO₂.

References

Mellouki, A., and Mu, Y. J., J. Photochem. Photobiol. A-Chem., 157, 295-300, 2003.