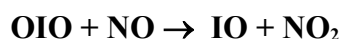


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx23

Website: <http://iupac.pole-ether.fr> See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

This data sheet last evaluated: 29th March 2006 (with no revision of preferred values).



$$\Delta H^\circ = -17.9 \text{ kJ mol}^{-1}$$

## Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$7.6 \times 10^{-13} \exp((607 \pm 128)/T)$ $(6.0 \pm 1.1) \times 10^{-12}$	235-320 298	Plane et al., 2006	PLP-CRDS (a)

## Comments

- (a) OIO formed in self-reaction of IO, produced by 193 nm photolysis of  $\text{N}_2\text{O}$  in the presence of  $\text{CF}_3\text{I}$ . The rate coefficient  $k$  was determined from the decay of OIO in the presence of excess NO. [OIO] measured by time resolved cavity ring-down spectroscopy (CRDS) at 567.808 nm.  $k$  was independent of pressure in the range 27 – 96 mbar at 300 K.

## Preferred Values

$$k = 6.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 1.1 \times 10^{-12} \exp(542/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over range } 240 - 320 \text{ K.}$$

### Reliability

$$\Delta \log k = \pm 0.3 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 250$$

### Comments on Preferred Values

The single experimental study provides well defined rate constants over the given pressure and temperature range, despite the complex source chemistry for the OIO radical. The observed rate constants and their temperature and pressure dependence were well reproduced by quantum chemical and RRKM calculations using a potential surface with a weakly bound OIONO intermediate which dissociates into IO +  $\text{NO}_2$  products. Even at 1 bar pressure significant formation of OIONO is not predicted to occur. The authors recommend the expression:  $(1.1 \pm 0.4) \times 10^{-12} \exp((542 \pm 130)/T)$  for  $k$  ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) at 1 bar, taking account of experimental uncertainties and the theoretical analysis, which is adopted for the preferred value for formation of IO +  $\text{NO}_2$  all pressures.

## References

Plane, J. M. C., Joseph, D. M., Allan, B. J., Ashworth, S. H., and Francisco, J. S.:  
Phys.Chem.A., 110, 93, 2006.