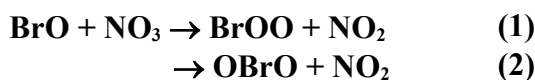


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iBrOx15

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 updated: 6<sup>th</sup> June 2007.



$$\Delta H^\circ (1) = -52 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ (2) = 3.5 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i> (0.3 - 3.0) $\times 10^{-12}$	298	Mellouki et al., 1989	DF-EPR (a)

### Comments

- (a) The decays of Br atoms and BrO radicals were monitored by EPR. Computer simulations of the results were carried out with a mechanism consisting of five reactions.

### Preferred Values

$$k = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

#### Reliability

$$\Delta \log k = \pm 0.5 \text{ at } 298 \text{ K.}$$

#### Comments on Preferred Values

The preferred value is based on the room temperature results Mellouki et al. (1989). This study (Mellouki et al., 1989) using the discharge flow-EPR technique, is the only experimental study of this reaction to date. The preferred value is the geometric mean of the upper and lower limits (Mellouki et al., 1989) which are encompassed within the stated uncertainty factor. The Br-O<sub>2</sub> bond is very weak and the bond energy has been estimated by Blake et al. (1970) to be 4 kJ mol<sup>-1</sup>. The product BrOO will therefore quickly decompose to yield Br + O<sub>2</sub>. There is no evidence for the second channel producing OBrO, which is slightly endothermic.

### References

Blake, J. A., Browne, R. J., and Burns, G.: J. Chem. Phys., 53, 3320, 1970.

Mellouki, A., Poulet, G., Le Bras, G., Singer, R., Burrows, J. P., and Moortgat, G. K.: J. Phys. Chem., 93, 8017, 1989.