

Correction to "Pressure-Dependent I Atom Yield in the Reaction of CH₂I with O₂ Shows a Remarkable Apparent Third-Body Efficiency for O₂"

Haifeng Huang, Brandon Rotavera, Arkke J. Eskola, and Craig A. Taatjes*

Combustion Research Facility, Mailstop 9055, Sandia National Laboratories, Livermore, California 94551-0969, United States J. Phys. Chem. Lett. 2012, 3 (22), 3399–3403. DOI: 10.1021/jz301585c

Supporting Information

In a recent publication, we reported an anomalously large apparent third-body efficiency of O_2 in quenching the I atom yield in the reaction of CH_2I with O_2 . Since that Letter appeared, other researchers have investigated the third-body efficiency of O_2 relative to N_2 and found no such anomaly. We have therefore reinvestigated the apparent collision efficiency of helium, O_2 , N_2 , and SF_6 in stabilizing CH_2IOO in the reaction of $CH_2I + O_2$ and now find no remarkably larger stabilization efficiency of O_2 than that of N_2 . The error in the initial report was caused by an incorrect treatment of the instrumental response function of the detection system in previous data processing, as described in detail in the accompanying Supporting Information. We deeply regret this error and apologize to those who have been misled by its erroneous conclusion.

Measurement of third-order rate constants using a correct procedure yields, with 1σ error, $k_{\rm He}=(1.5\pm0.2)\times10^{-31}, k_{\rm O2}=(1.8\pm0.2)\times10^{-31}, k_{\rm N2}=(3.8\pm0.7)\times10^{-31},$ and $k_{\rm SF6}=(7.0\pm2.0)\times10^{-31}$ cm 6 molecule $^{-2}$ s $^{-1}$ at 298 K, on the same order as those reported for similar systems 2 (see the original paper for other references). The extrapolated yield of the I + Criegee channel at tropospheric conditions (298 K and 760 Torr air) is 0.15 \pm 0.03 (1σ) , in excellent agreement with the work of Stone et al. 2

ASSOCIATED CONTENT

Supporting Information

Supplementary text, Figures 1–3. This material is available free of charge via the Internet at http://pubs.acs.org.

REFERENCES

- (1) Huang, H.; Eskola, A. J.; Taatjes, C. A. Pressure-Dependent I-Atom Yield in the Reaction of CH₂I with O₂ Shows a Remarkable Apparent Third-Body Efficiency for O₂. J. Phys. Chem. Lett. **2012**, 3, 3399–3403.
- (2) Stone, D.; Blitz, M.; Daubney, L.; Ingham, T.; Seakins, P. CH₂OO Criegee Biradical Yields Following Photolysis of CH₂I₂ in O₂. *Phys. Chem. Chem. Phys.* **2013**, *15*, 19119–19124.