# Reply to Comment on "Inverse Kinetic Isotope Effect in the Reaction of Atomic Chlorine with $C_2H_4$ and $C_2D_4$"

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Our measurements were directed to elucidating the magnitude and direction for the kinetic isotope effect for the reaction of Cl with $C_2H_4$ and $C_2D_4$, respectively, and hence on the ratio of the rate constants. Table 1 summarizes the individual relative rate data for which the weighted average was reported earlier.[1] It is seen that typical $2\sigma$ values in individual RR experiments were ~20−40%. Because of this, the standard deviation for the limited number of runs in He is also large (27%). Given these larger errors and the limited number of relative rate runs in He, deriving quantitative values for the third body efficiency of $N_2$ versus He from these data is not appropriate and does not affect the conclusion of the paper that there is an inverse kinetic isotope effect of approximately 3 for the Cl + $C_2H_4$/$C_2D_4$ reaction.

**TABLE 1: Relative Rate Data for the Reaction of Chlorine Atoms with $C_2H_4$ at Room Temperature Using $CH_4$ as the Reference Compound**

| $[C_2H_4]$ ($10^{14}$ molecules $cm^{-3}$) | $[CH_4]$ ($10^{15}$ molecules $cm^{-3}$) | $[Cl_2]$ ($10^{15}$ molecules $cm^{-3}$) | $k_{eth}/k_{CH_4} \pm 2\sigma$[a] | weighted av $k_{eth}/k_{CH_4} \pm 2\sigma$[b] |
|---|---|---|---|---|
| | | In $N_2$ | | |
| 3.0 | 1.2 | 1.2 | $3.10 \pm 0.84$ | |
| 2.0 | 1.3 | 1.1 | $2.96 \pm 0.82$ | |
| 1.5 | 1.2 | 1.2 | $2.52 \pm 0.76$ | $2.87 \pm 0.32$ |
| 5.9 | 1.2 | 1.2 | $3.53 \pm 1.16$ | |
| 1.5 | 1.2 | 1.2 | $2.63 \pm 0.58$ | |
| 2.4 | 1.2 | 1.2 | $3.10 \pm 0.78$ | |
| | | In He | | |
| 2.2 | 1.8 | 1.6 | $2.68 \pm 1.02$ | |
| 3.2 | 1.3 | 1.3 | $2.97 \pm 1.15$ | $2.80 \pm 0.76$ |

[a] Statistical errors only taking into account errors in both the $C_2H_4$ and $CH_4$ concentrations as described in ref 2; six runs were carried out in $N_2$ rather than seven as reported.[1] [b] Standard deviation calculated from $\sigma^2 = 1/\sum(1/\sigma_I^2)$.[3]

## References and Notes

(1) Stutz, J.; Ezell, M. J.; Finlayson-Pitts, B. J. *J. Phys. Chem. A* **1997**, *101*, 9187.

(2) Brauers, T.; Finlayson-Pitts, B. J. *Int. J. Chem. Kinet.* **1997**, *29*, 665.

(3) Bevington, P. R. *Data Reduction and Error Analysis for the Physical Sciences*; McGraw-Hill: New York, 1969.

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