CHAPTER 3 – SUPPLEMENT 2

Evaluation of Atmospheric Loss Processes: $O(^1D)$ Kinetics Supplement

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Rate coefficients for the reaction of $O(^1D)$ with the compounds included in the SPARC Lifetime report have received various amounts of attention. Possible exothermic $O(^1D)$ reaction pathways include (1) collisional (physical) quenching of $O(^1D)$ to ground state oxygen atoms, $O(^3P)$, (2) abstraction or addition-elimination, and (3) reactive quenching to form $O(^3P)$ and products other than the reactant, including stable and radical species. The figures included in this supplement contain (1) a summary of the available literature data for each reaction, (2) the SPARC recommendation for the overall reaction, $O(^1D)$ loss, (3) the reaction yield, i.e., the fraction of the overall reaction that leads to reactant loss, and (4) the 2σ uncertainty range in the recommended reaction-rate coefficient for $O(^1D)$ loss.

The uncertainties quoted herein follow the format given in the NASA/JPL[1] data evaluation where $f(\mathrm{T})$ is the 1σ estimated uncertainty in the rate coefficient, $k(\mathrm{T})$ at temperature T

$$f(\mathrm{T}) = f(298\ \mathrm{K})\ \exp\left(\left|g\left(\frac{1}{\mathrm{T}} - \frac{1}{298}\right)\right|\right)$$

$f(298\ \mathrm{K})$ is the 1σ estimated uncertainty in the room-temperature rate coefficient, $k(298\ \mathrm{K})$, and g is a parameter used to describe the possible increase in uncertainty at temperatures other than 298 K.

The basis for the recommended rate coefficients given here is described in the footnotes of Table 3.2.

Reference

(1) Sander, S., J. Abbatt, J. R. Barker, J. B. Burkholder, R. R. Friedl, D. M. Golden, R. E. Huie, C. E. Kolb, M. J. Kurylo, G. K. Moortgat, V. L. Orkin, and P. H. Wine, *Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 17, JPL Publication 10-6*, Jet Propulsion Laboratory, California Institute of Technology, 2011.

Table 3.2. Reaction-rate coefficients, reaction yields, and estimated uncertainties for the O(^{1}D) + compound gas-phase reactions.*

Compound	Chemical Formula	Temperature Range (K) **	*A* *	*E*/R (K)	*k*(298 K) *	*f*(298 K)	*g*	Reaction Yield	Footnotes
1. CFC−11	CCl_3F	173 – 372	230	0	230	1.10	0	0.79 ± 0.04	1,2,3
2. CFC−12	CCl_2F_2	173 – 373	140	-25	157	1.15	0	0.76 ± 0.06	1,2,3,4
3. CFC−113	CCl_2FCClF_2	217 – 373	232	0	232	1.1	0	0.80 ± 0.04	2,3,4,5
4. CFC−114	$CClF_2CClF_2$	217 – 373	130	-25	142	1.1	0	0.80 ± 0.10	2,3,4,5
5. CFC−115	CF_3CClF_2	217 – 373	54	-30	60	1.15	0	0.84 ± 0.07	2,3,4
6. Carbon Tetrachloride	CCl_4	203 – 343	330	0	330	1.15	0	0.79 ± 0.04	1,2
7. Nitrous Oxide	N_2O	195 – 719	119	-20	127	1.1	25	0.39 ($N_2 + O_2$) 0.61 (2NO)	6
8. Halon−1202	CBr_2F_2	297	220	*0*	220	1.2	50	0.45 ± 0.06	6
9. Halon−1211	$CBrClF_2$	297	150	*0*	150	1.2	50	0.65 ± 0.04	6
10. Halon−1301	$CBrF_3$	297	100	*0*	100	1.2	50	0.40 ± 0.08	6
11. Halon−2402	$CBrF_2CBrF_2$	297	160	*0*	160	1.2	50	0.75 ± 0.07	6
12. Methane	CH_4	198 – 369	175	0	175	1.15	25	$1.0^{+0}_{-0.002}$	6
13. Methyl Chloroform	CH_3CCl_3	298	*325*	*0*	*325*	1.4	*0*	*0.9*	7,8
14. Methyl Chloride	CH_3Cl	298	260	*0*	260	1.3	50	0.91 ± 0.06	7,9
15. Methyl Bromide	CH_3Br	297	180	*0*	180	1.15	50	$1.0^{+0}_{-0.07}$	6
16. HCFC−22	$CHClF_2$	173 – 373	102	0	102	1.07	0	0.72 ± 0.06	2,3,4
17. HCFC−141b	CH_3CCl_2F	297	260	*0*	260	1.2	50	0.70 ± 0.05	6
18. HCFC−142b	CH_3CClF_2	217 – 373	200	0	200	1.1	0	0.75 ± 0.05	2,3,4
19. HFC−23	CHF_3	217 –372	8.7	-30	9.6	1.05	0	0.25 ± 0.05	2,3,4
20. HFC−32	CH_2F_2	298	51	*0*	51	1.2	50	0.30 ± 0.10	6
21. HFC−125	CHF_2CF_3	217 – 373	9.5	-25	10.5	1.07	0	0.70 ± 0.09	2,4,10
22. HFC−134a	CH_2FCF_3	297	49	*0*	49	1.15	50	0.35 ± 0.06	6
23. HFC−143a	CF_3CH_3	217 – 373	56	-20	60	1.2	0	0.65 ± 0.05	2,3,4
24. HFC−152a	CH_3CHF_2	297	175	*0*	175	1.2	50	0.55 ± 0.20	6
25. HFC−227ea	CF_3CHFCF_3	217 – 373	7.9	-70	10	1.1	0	0.72 ± 0.07	7,10
26. HFC−245fa	$CHF_2CH_2CF_3$	–	*150*	*0*	*150*	*1.3*	*0*	*0.5*	7
27. Nitrogen Trifluoride	NF_3	212 – 351	*20*	-44	*23*	*1.1*	*0*	$0.93^{+0.07}_{-0.21}$	2,4,11

Footnotes

* Estimated values are given in italics; *A* and *k*(298 K) are in units of 10^{-12} cm^3 $molecule^{-1}$ s^{-1}; $k(T) = A \exp(-E/RT)$.

** Temperature range of available experimental data considered in the evaluation of the reaction-rate coefficient parameters and uncertainty limits.

1. Reactive yields taken from Feierabend *et al.* (2010).
2. Estimated uncertainty parameters revised from values reported in JPL10-6.
3. Recommended kinetic parameters and uncertainties based on evaluation of studies included in JPL10-6 as well as Baasandorj *et al.* (2013).
4. Kinetic parameters revised from values reported in JPL10-6.
5. Kinetic parameters taken from Baasandorj *et al.* (2011) and Baasandorj *et al.* (2013).
6. Kinetic parameters taken from JPL10-6.
7. Not evaluated in JPL10-6.
8. Nilsson *et al*. (2012) report a room-temperature reactive-rate coefficient, obtained using a relative rate method, of $(2.93 \pm 1.2) \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} (1σ error limit). The total rate coefficient given in the table was calculated assuming a 0.9 reaction yield.
9. Rate coefficient is an average of the values reported by Matsumi *et al.* (1993) and Force and Wiesenfeld (1981). The reaction yield was taken from Force and Wiesenfeld (1981).
10. Kinetic parameters taken from Baasandorj *et al.* (2013).
11. The recommended *k*(298 K) for the overall reaction is an average of the values derived from Arrhenius fits to the data of Zhao *et al.* (2010) and Dillon *et al.* (2011) and the value reported by Baasandorj *et al.* (2012) at 296 K. The recommended Arrhenius parameters are derived from a fit to these data after normalization to *k*(298 K). The recommended reaction yield is an average of the values reported by Zhao *et al.* (0.99) and Baasandorj *et al.* (2012) (0.87 +0.13/-0.15). The reaction yield is expected to be independent of temperature.

References

Baasandorj, M., K. J. Feierabend, and J. B. Burkholder, Rate coefficients and ClO radical yields in the reaction of $O(^1D)$ with $CClF_2CCl_2F$, CCl_3CF_3, $CClF_2CClF_2$, and CCl_2FCF_3, *Int. J. Chem Kinet.*, *43*, 1-9, 2011.

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Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, $O(^1D)$ kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Dillon, T. J., L. Vereecken, A. Horowitz, V. Khamaganov, J. N. Crowley, and J. Lelieveld, Removal of the potent greenhouse gas NF_3 by reactions with the atmospheric oxidants $O(^1D)$, OH and O_3, *Phys. Chem. Chem. Phys.*, *13*, 18600-18608, 2011.

Feierabend, K. J., D. K. Papanastasiou, and J. B. Burkholder, ClO radical yields in the reaction of $O(^1D)$ with Cl_2, HCl, chloromethanes and chlorofluoromethanes, *J. Phys. Chem. A*, *114*, 12052-12061, 2010.

Force, A. P., and J. R. Wiesenfeld, Collisional deactivation of $O(^1D_2)$ by the halomethanes. direct determination of reaction efficiency, *J. Phys. Chem.*, *85*, 782-785, 1981.

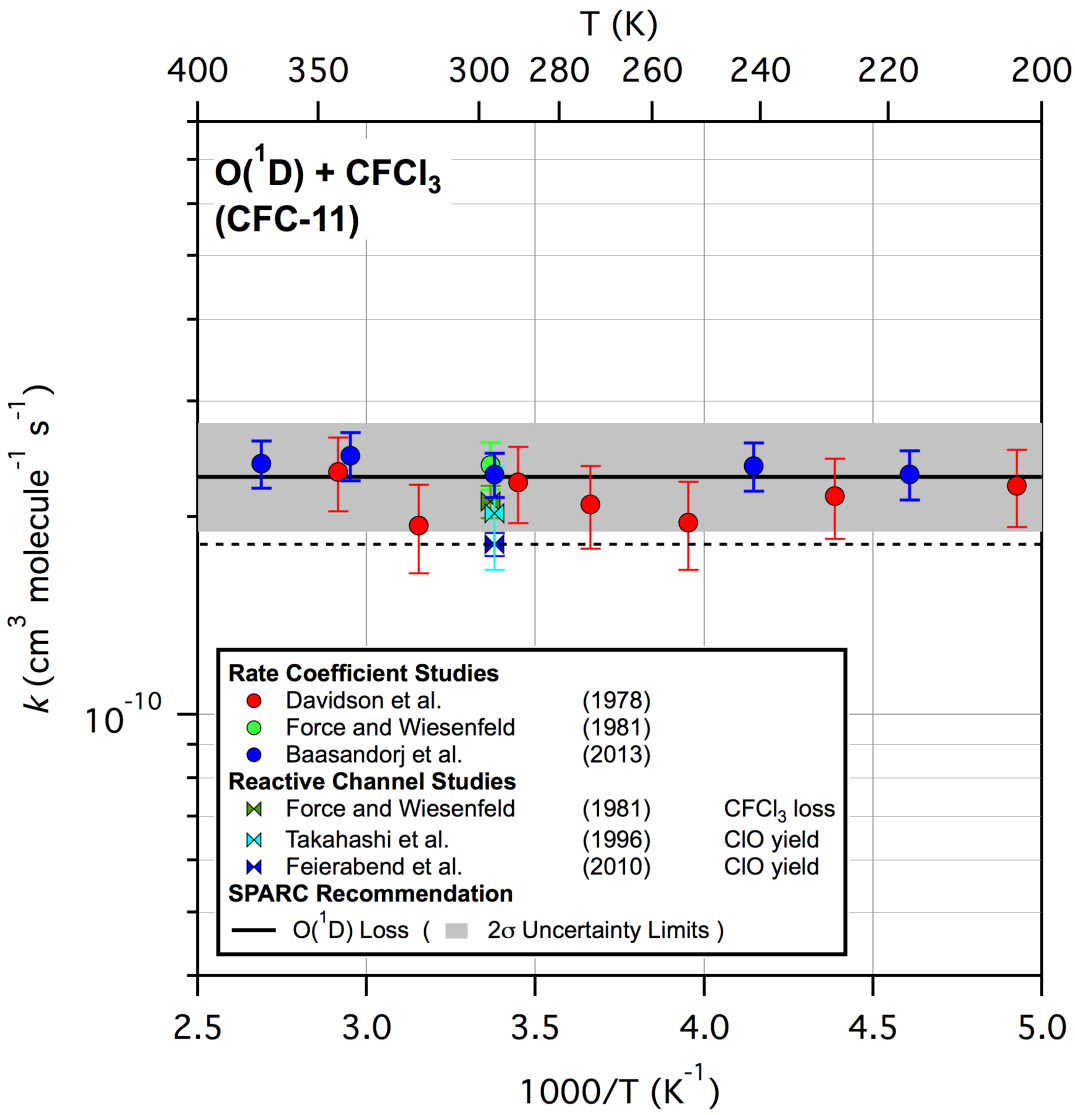
Matsumi, Y., K. Tonokura, Y. Inagaki, and M. Kawasaki, Isotopic branching ratios and translational energy release of H and D atoms in reaction of $O(^1D)$ atoms with alkanes and alkyl chlorides, *J. Phys. Chem.*, *97*, 6816-6821, 1993.

Nilsson, E. J. K., V. F. Andersen, O. J. Nielsen, and M. S. Johnson, Rate coefficients for the chemical reactions of CH_2F_2, $CHClF_2$, CH_2FCF_3 and CH_3CCl_3 with $O(^1D)$ at 298 K. *Chem. Phys. Lett.*, *554*, 27-32, 2012.

Sander, S. P., J. Abbatt, J. R. Barker, J. B. Burkholder, R. R. Friedl, D. M. Golden, R. E. Huie, C. E. Kolb, M. J. Kurylo, G. K. Moortgat, V. L. Orkin, and P. H. Wine, *Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 17, JPL Publication 10-6,* Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California, 2011, http://jpldataeval.jpl.nasa.gov.

Zhao, Z., P. L. Laine, J. M. Nicovich, and P. H. Wine, Reactive and non-reactive quenching of $O(^3P)$ by the potent greenhouse gases SO_2F_2, NF_3, and SF_5CF_3, *Proc. Nat. Acad. Sci.*, *107*, 6610-6615, 2010.

1. $CFCl_3$ (CFC-11)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 2.3 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 2.3 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Unchanged from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.10$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.79 ± 0.04

Revised from JPL10-6

References

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, O(^{1}D) kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

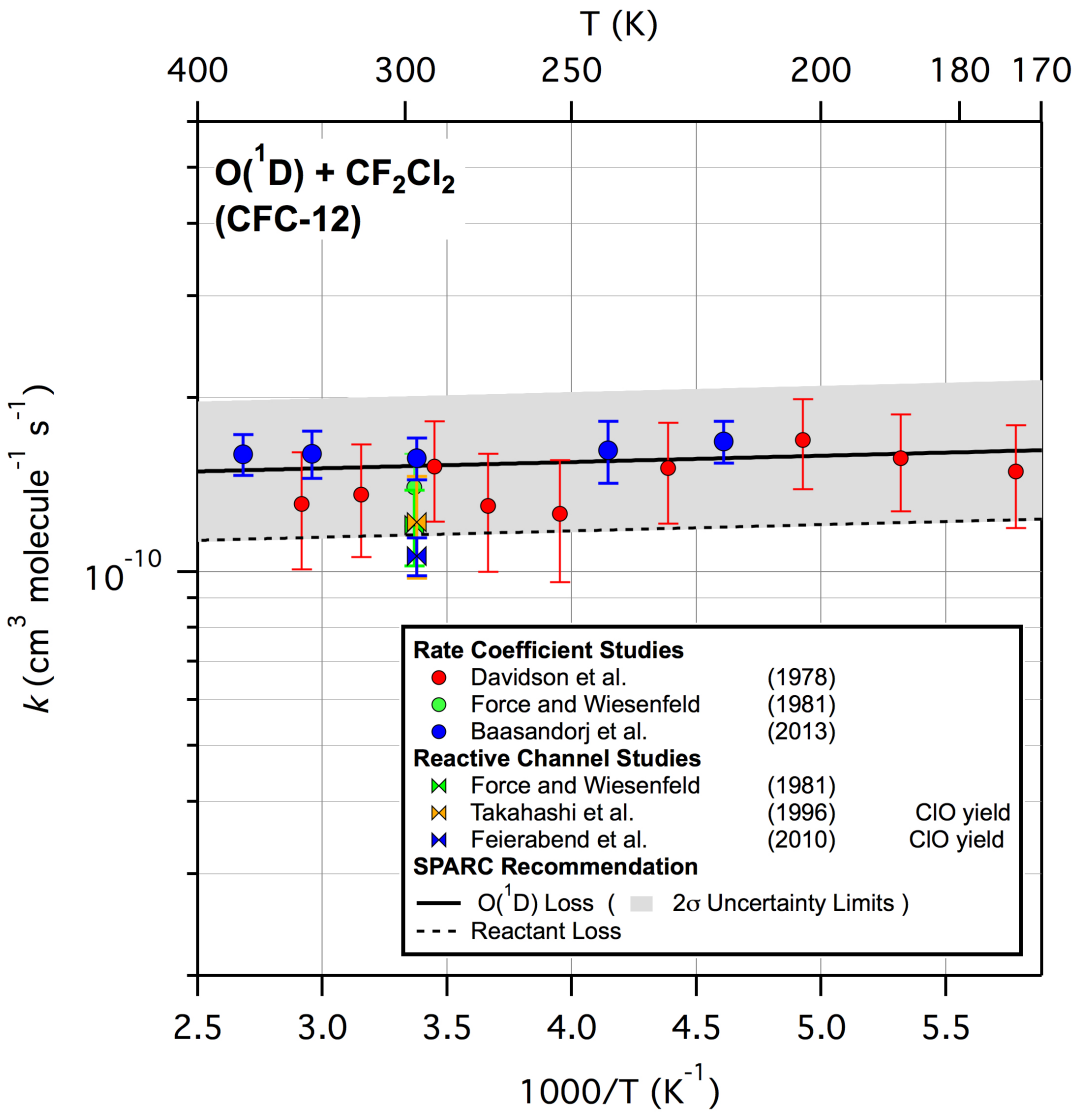
Davidson, J. A., H. I. Schiff, T. J. Brown, and C. J. Howard, Temperature dependence of the rate constants for reactions of O(^{1}D) atoms with a number of halocarbons, *J. Chem. Phys.*, *69*, 4277-4279, 1978.

Feierabend, K. J., D. K. Papanastasiou, and J. B. Burkholder, ClO radical yields in the reaction of $O(^1D)$ with Cl_2, HCl, chloromethanes and chlorofluoromethanes, *J. Phys. Chem. A*, *114*, 12052-12061, 2010.

Force, A. P., and J. R. Wiesenfeld, Collisional deactivation of $O(^1D_2)$ by the halomethanes. direct determination of reaction efficiency, *J. Phys. Chem.*, *85*, 782-785, 1981.

Takahashi, K., R. Wada, Y. Matsumi, and M. Kawasaki, Product branching ratios for $O(^3P)$ atom and ClO radical formation in the reactions of $O(^1D)$ with chlorinated compounds, *J. Phys. Chem.*, *100*, 10145-10149, 1996.

2. CF_2Cl_2 (CFC-12)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 1.4 \times 10^{-10} \exp(25/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.57 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.15$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.76 ± 0.06

Revised from JPL10-6

References

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, O(^{1}D) kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

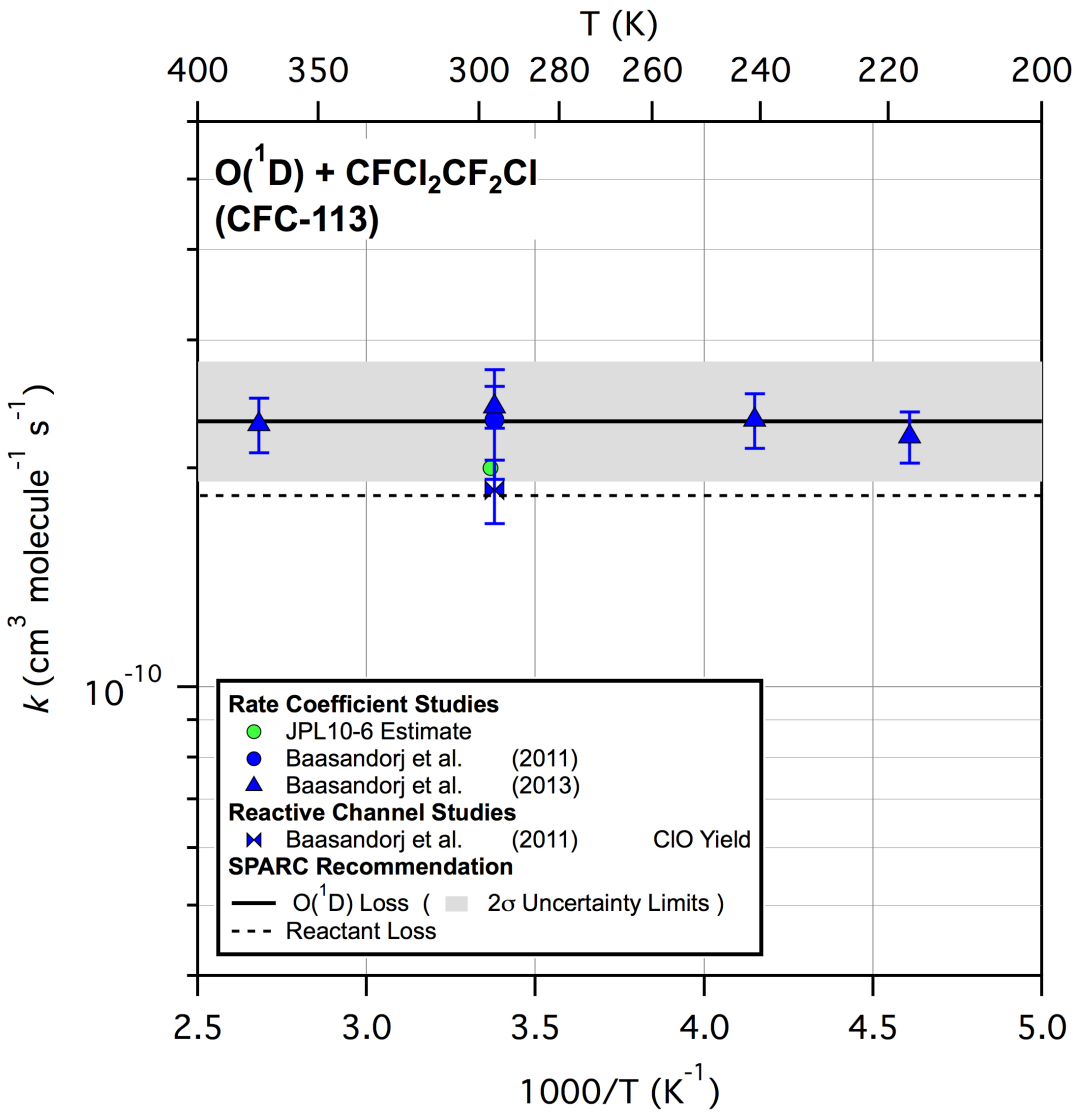
Davidson, J. A., H. I. Schiff, T. J. Brown, and C. J. Howard, Temperature dependence of the rate constants for reactions of O(^{1}D) atoms with a number of halocarbons, *J. Chem. Phys.*, *69*, 4277-4279, 1978.

Feierabend, K. J., D. K. Papanastasiou, and J. B. Burkholder, ClO radical yields in the reaction of $O(^1D)$ with Cl_2, HCl, chloromethanes and chlorofluoromethanes, *J. Phys. Chem. A*, *114*, 12052-12061, 2010.

Force, A. P., and J. R. Wiesenfeld, Collisional deactivation of $O(^1D_2)$ by the halomethanes. direct determination of reaction efficiency, *J. Phys. Chem.*, *85*, 782-785, 1981.

Takahashi, K., R. Wada, Y. Matsumi, and M. Kawasaki, Product branching ratios for $O(^3P)$ atom and ClO radical formation in the reactions of $O(^1D)$ with chlorinated compounds, *J. Phys. Chem.*, *100*, 10145-10149, 1996.

3. $CF_2ClCFCl_2$ (CFC-113)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 2.32 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 2.32 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.1$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.80 ± 0.04

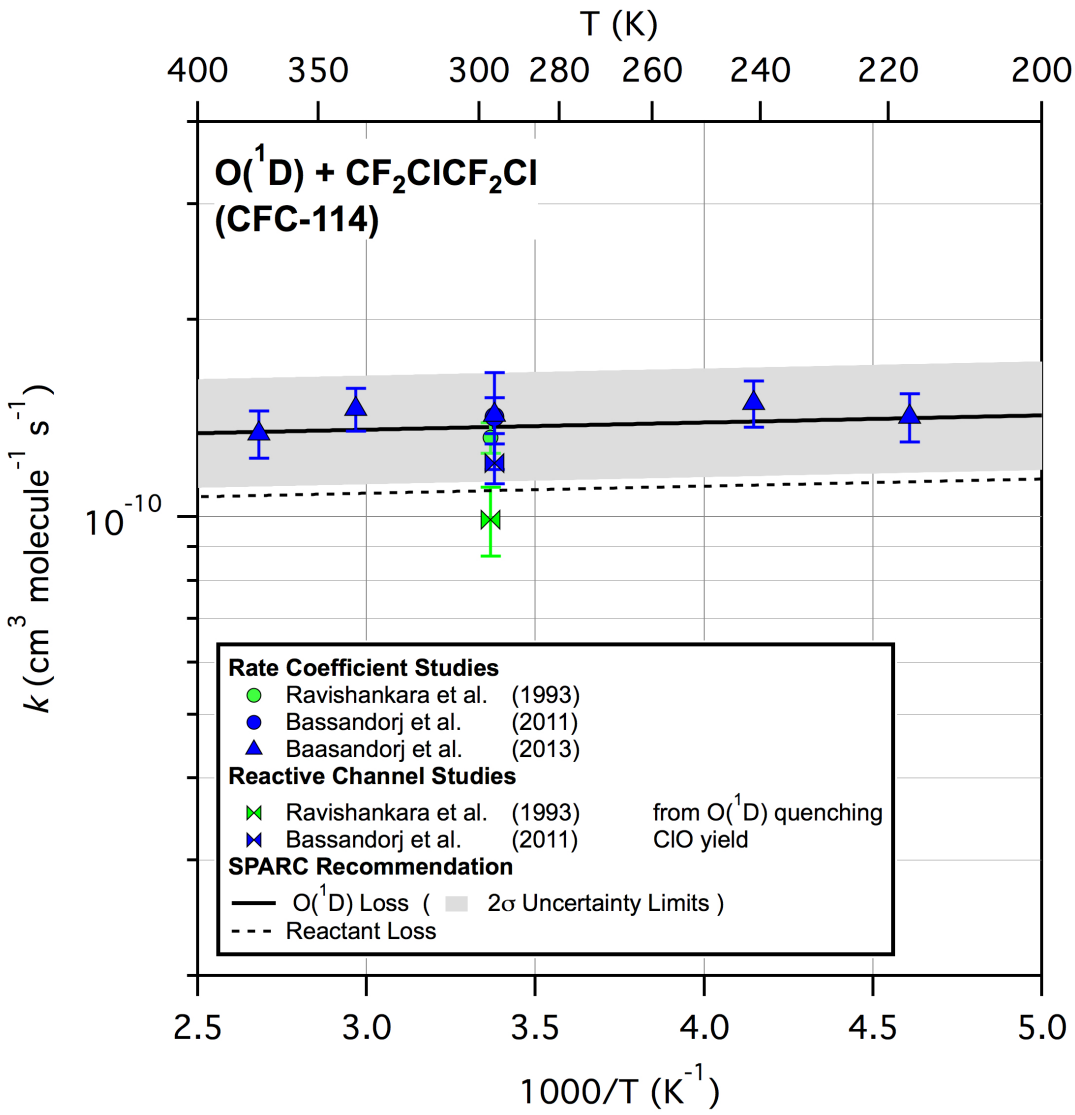
Revised from JPL10-6

References

Baasandorj, M., K. J. Feierabend, and J. B. Burkholder, Rate coefficients and ClO radical yields in the reaction of O(^{1}D) with $CClF_2CCl_2F$, CCl_3CF_3, $CClF_2CClF_2$, and CCl_2FCF_3, *Int. J. Chem Kinet.*, *43*, 1-9, 2011.

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, O(^{1}D) kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

4. CF_2ClCF_2Cl (CFC-114)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.3 \times 10^{-10} \exp(25/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.42 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.1$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.80 ± 0.10

Revised from JPL10-6

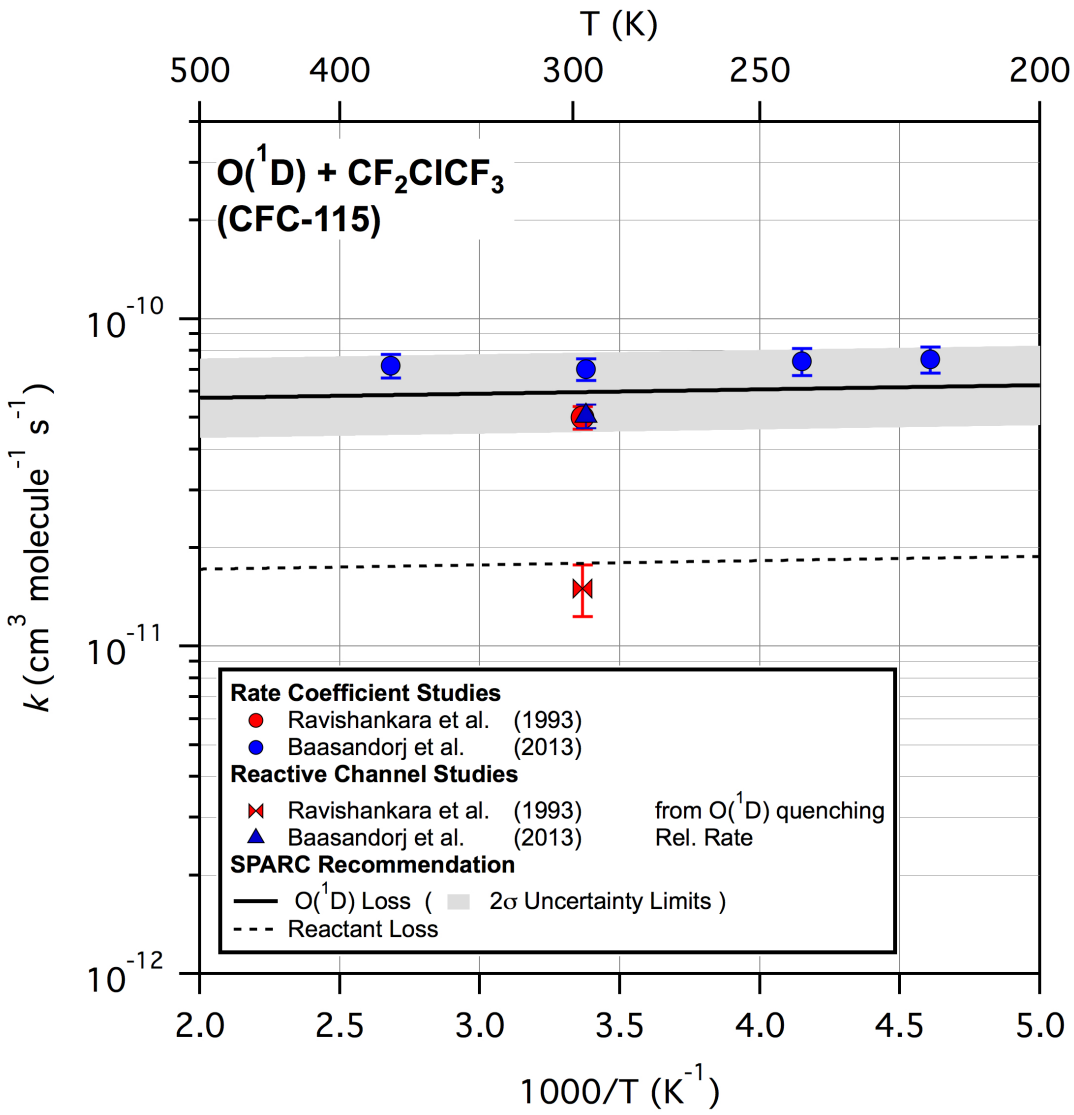
References

Baasandorj, M., K. J. Feierabend, and J. B. Burkholder, Rate coefficients and ClO radical yields in the reaction of $O(^1D)$ with $CClF_2CCl_2F$, CCl_3CF_3, $CClF_2CClF_2$, and CCl_2FCF_3, *Int. J. Chem Kinet.*, *43*, 1-9, 2011.

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, $O(^1D)$ kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Ravishankara, A. R., S. Solomon, A. A. Turnipseed, and R. F. Warren, Atmospheric lifetimes of long-lived halogenated species, *Science*, *259*, 194-199, 1993.

5. CF_3CF_2Cl (CFC-115)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 5.4 \times 10^{-11} \exp(30/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 6.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.15$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.30 ± 0.07

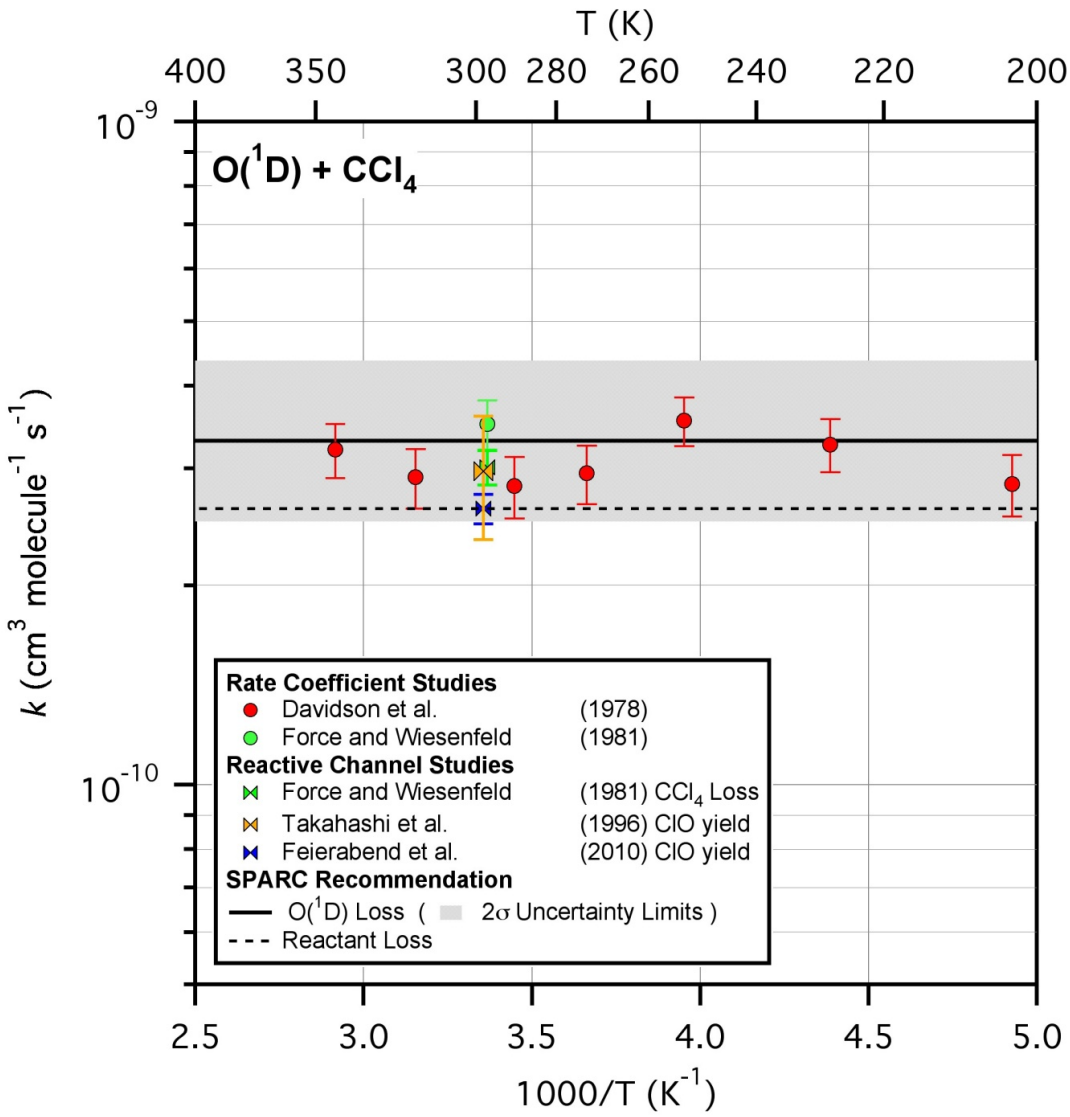
Revised from JPL10-6

References

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, $O(^1D)$ kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Ravishankara, A. R., S. Solomon, A. A. Turnipseed, and R. F. Warren, Atmospheric lifetimes of long-lived halogenated species, *Science*, *259*, 194-199, 1993.

6. CCl_4 (Carbon Tetrachloride)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 3.3 \times 10^{-10} \exp(0/T)$ cm^3 $molecule^{-1}$ s^{-1}

$k(298\ K) = 3.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

Unchanged from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.15$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.79 ± 0.04

Revised from JPL10-6

References

Davidson, J. A., H. I. Schiff, T. J. Brown, and C. J. Howard, Temperature dependence of the rate constants for reactions of $O(^1D)$ atoms with a number of halocarbons, *J. Chem. Phys.*, *69*, 4277-4279, 1978.

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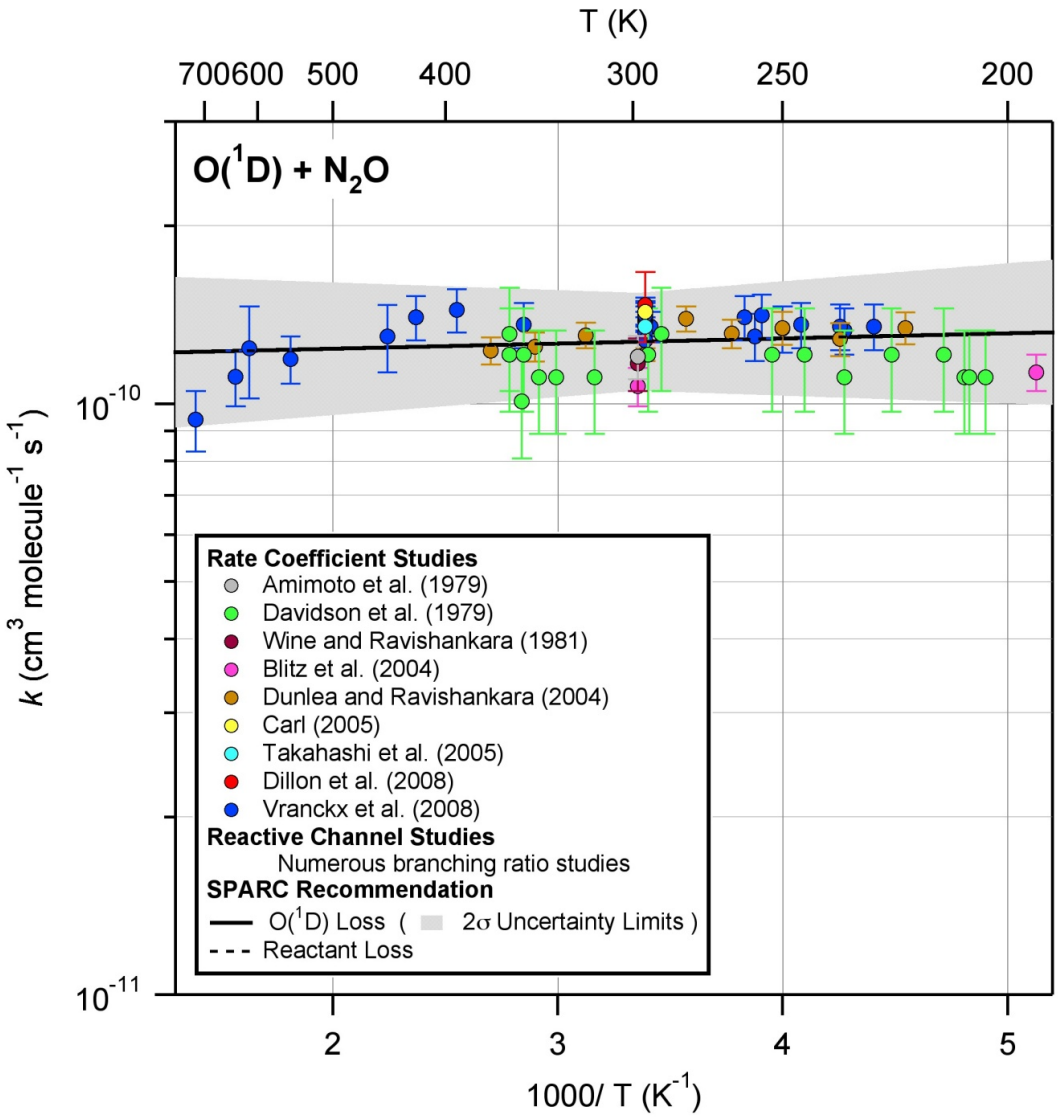
Takahashi, K., R. Wada, Y. Matsumi, and M. Kawasaki, Product branching ratios for $O(^3P)$ atom and ClO radical formation in the reactions of $O(^1D)$ with chlorinated compounds, *J. Phys. Chem.*, *100*, 10145-10149, 1996.

7. N_2O



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.19 \times 10^{-10} \exp(20/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.27 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.10$

$g = 25$

Recommended Reactive Yield: Reactant Loss

0.39 ($N_2 + O_2$)

0.61 (2NO)

All parameters unchanged from JPL10-6

References

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Blitz, M. A., T. J. Dillon, D. E. Heard, M. J. Pilling, and I. D. Trought, Laser induced fluorescence studies of the reactions of $O(^1D_2)$ with N_2, O_2, N_2O, CH_4, H_2, CO_2, Ar, Kr and n-C_4H_{10}, *Phys. Chem. Chem. Phys.*, *6*, 2162-2171, 2004.

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Takahashi, K., Y. Takeuchi, and Y. Matsumi, Rate constants of the $O(^1D)$ reactions with N_2, O_2, N_2O, and H_2O at 295 K, *Chem. Phys. Lett.*, *410*, 196-200, 2005.

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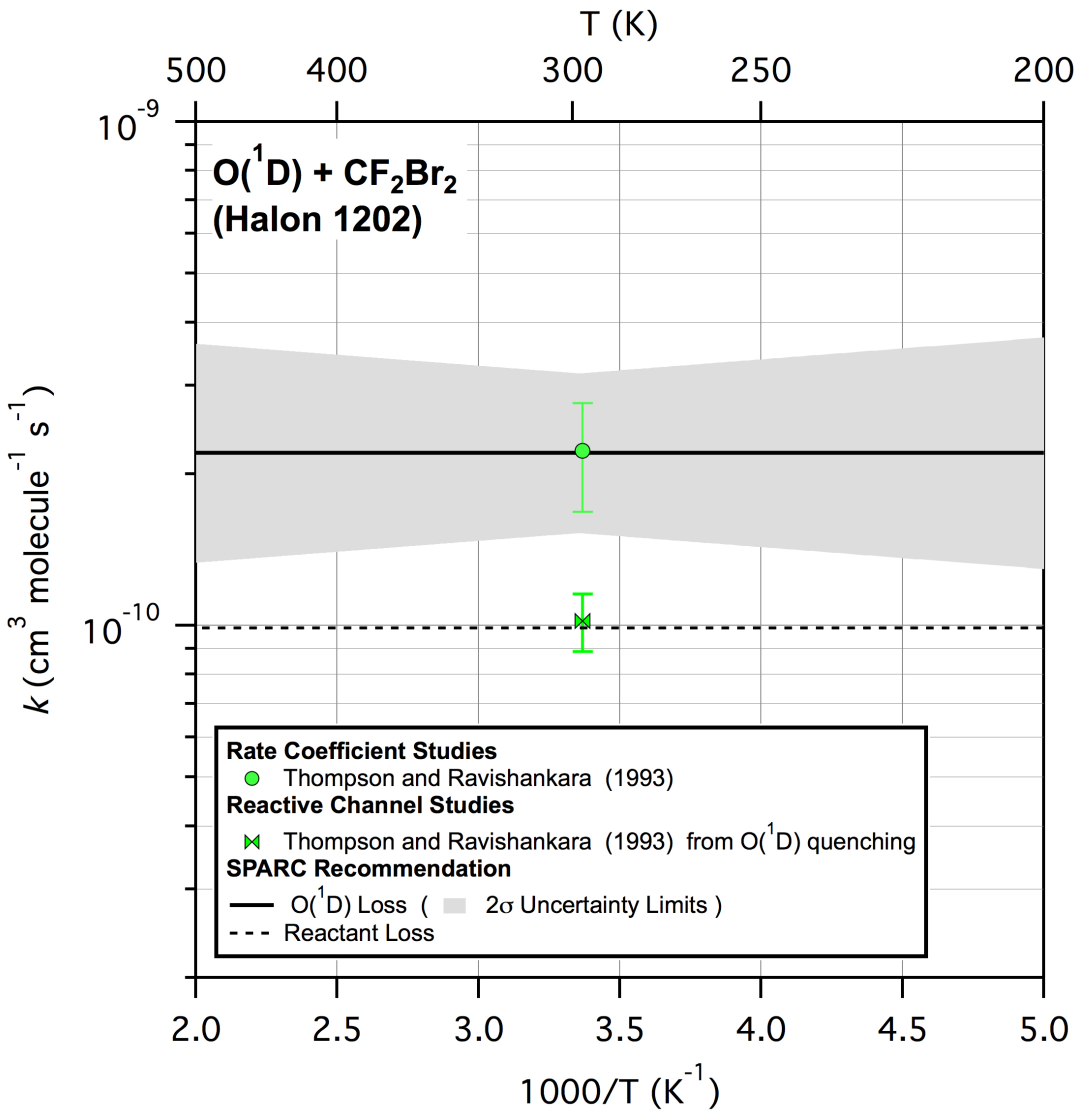
Vranckx, S., J. Peeters, and S. A. Carl, Absolute rate constant and $O(^3P)$ yield for the $O(^1D)$ + N_2O reaction in the temperature range 227 K to 719 K, *Atmos. Chem. Phys.*, *8*, 6261-6272, 2008.

8. CF_2Br_2 (Halon-1202)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 2.2 \times 10^{-10} \exp(0/T)$ cm^3 $molecule^{-1}$ s^{-1}

$k(298\ K) = 2.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

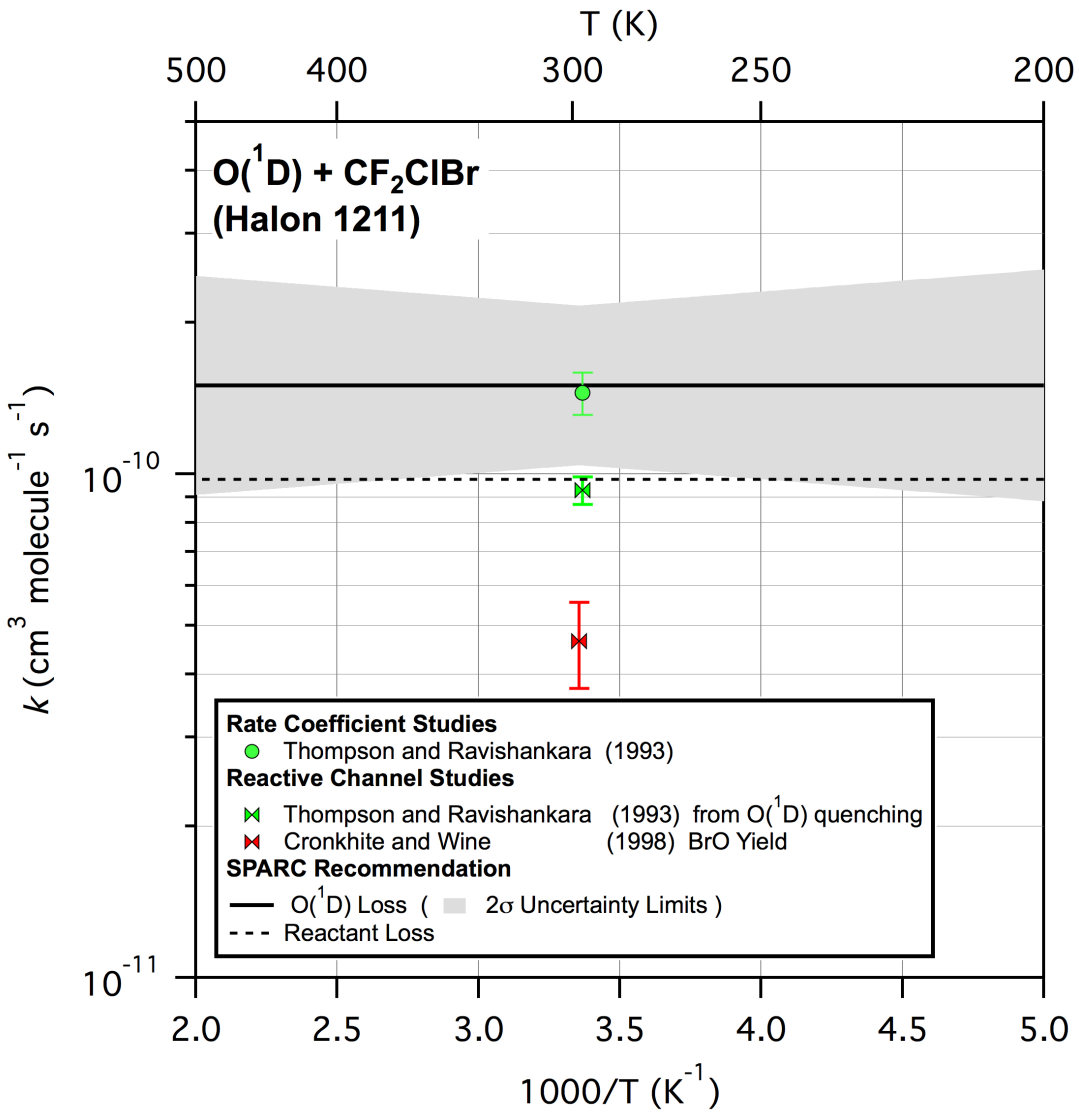
0.45 ± 0.06

All parameters unchanged from JPL10-6

Reference

Thompson, J. E., and A. R. Ravishankara, Kinetics of $O(^1D)$ reactions with bromocarbons, *Int. J. Chem. Kinet.*, *25*, 479-487, 1993.

9. CF_2ClBr (Halon-1211)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.5 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\text{ K}) = 1.5 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\text{ K}) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.65 ± 0.04

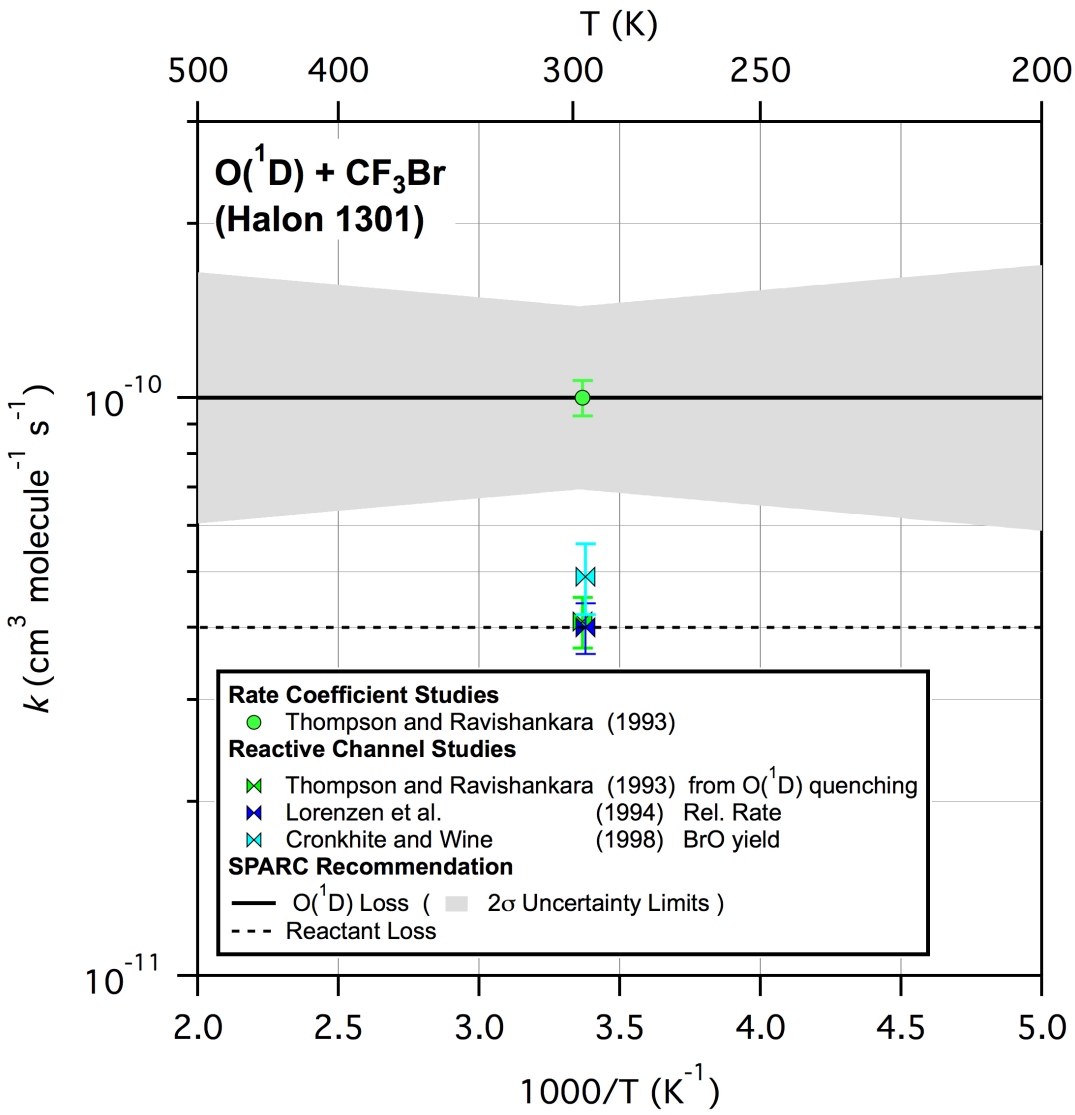
All parameters unchanged from JPL10-6

References

Cronkhite, J. M., and P. H. Wine, Branching ratios for BrO production from reactions of $O(^1D)$ with HBr, CF_3Br, CH_3Br, CF_2ClBr, and CF_2HBr, *Int. J. Chem. Kinet.*, *30,* 555-563, 1998.

Thompson, J. E., and A. R. Ravishankara, Kinetics of $O(^1D)$ reactions with bromocarbons, *Int. J. Chem. Kinet.*, *25*, 479-487, 1993.

10. CF_3Br (Halon-1301)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.0 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.0 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.40 ± 0.08

All parameters unchanged from JPL10-6

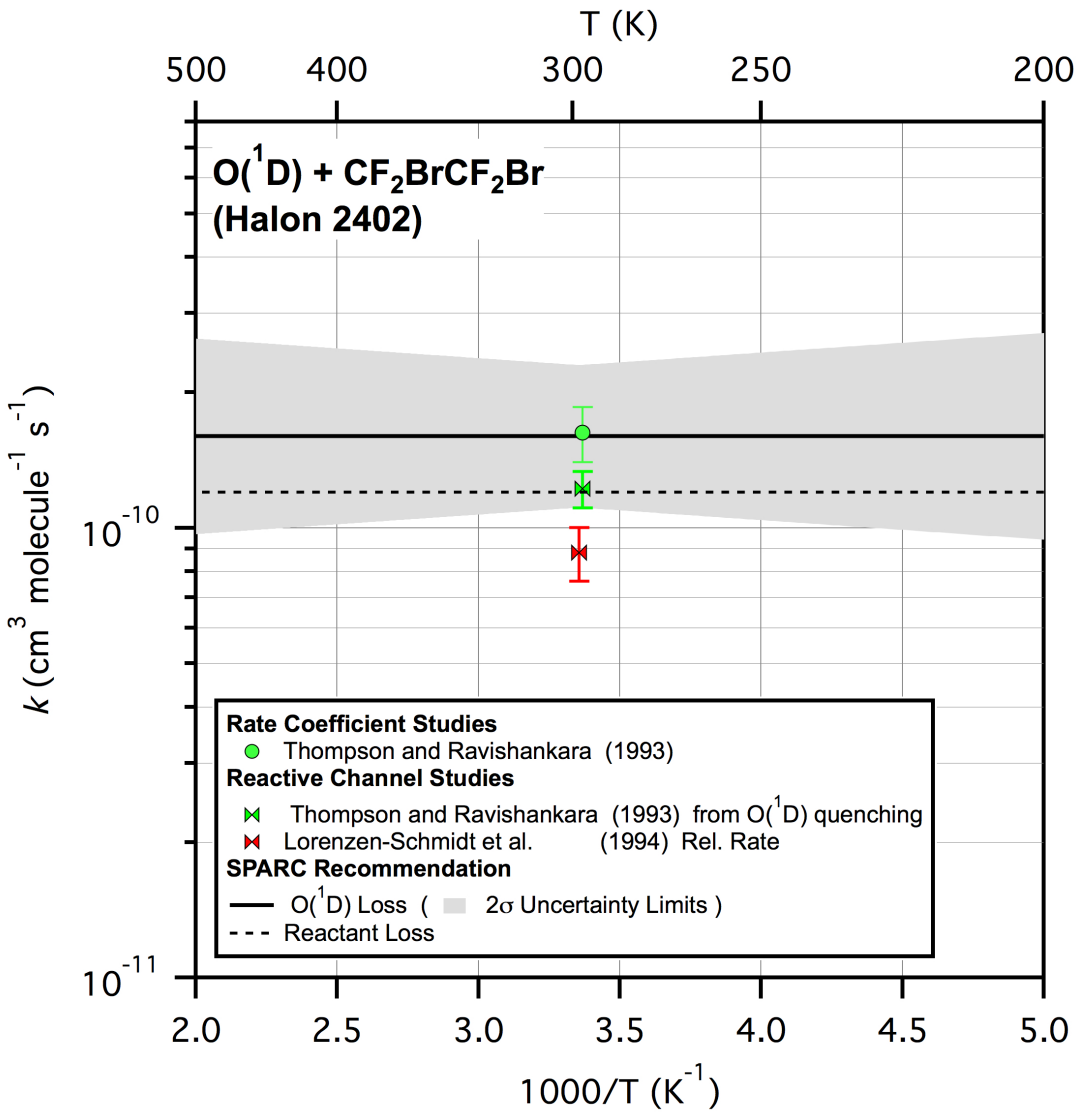
References

Cronkhite, J. M., and P. H. Wine, Branching ratios for BrO production from reactions of $O(^1D)$ with HBr, CF_3Br, CH_3Br, CF_2ClBr, and CF_2HBr, *Int. J. Chem. Kinet.*, *30,* 555-563, 1998.

Lorenzen-Schmidt, H., R. Weller, and O. Schrems, Kinetics and mechanisms of the reactions of $O(^1D)$-atoms with CF_3Br and CF_3BrCF_2Br in the gas phase and in solid Argon matrices, *Ber. Bunsenges. Phys. Chem.*, *98*, 1622-1629, 1994.

Thompson, J. E., and A. R. Ravishankara, Kinetics of $O(^1D)$ reactions with bromocarbons, *Int. J. Chem. Kinet.*, *25*, 479-487, 1993.

11. CF_2BrCF_2Br (Halon-2402)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.6 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\text{ K}) = 1.6 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\text{ K}) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.75 ± 0.07

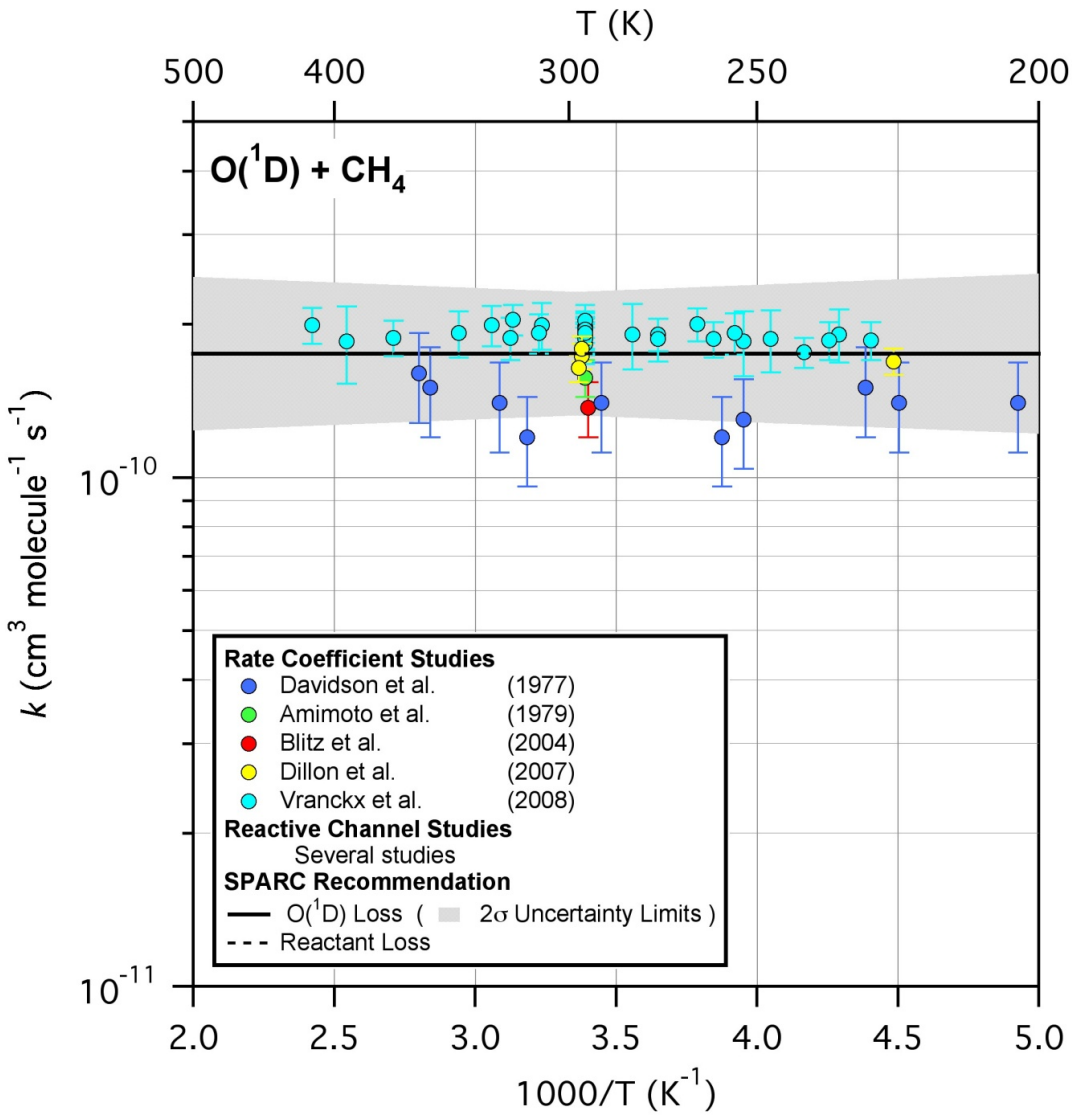
All parameters unchanged from JPL10-6

References

Lorenzen-Schmidt, H., R. Weller, and O. Schrems, Kinetics and mechanisms of the reactions of $O(^1D)$-atoms with CF_3Br and CF_3BrCF_2Br in the gas phase and in solid Argon matrices, *Ber. Bunsenges. Phys. Chem.*, *98*, 1622-1629, 1994.

Thompson, J. E., and A. R. Ravishankara, Kinetics of $O(^1D)$ reactions with bromocarbons, *Int. J. Chem. Kinet.*, *25*, 479-487, 1993.

12. CH_4 (Methane)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 1.75 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.75 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.15$

$g = 25$

Recommended Reactive Yield: Reactant Loss

1.0 +0/-0.002

All parameters unchanged from JPL10-6

References

Amimoto, S. T., A. P. Force, R. G. Gulotty, Jr., and J. R. Wiesenfeld, Collisional deactivation of O(2^{1}D$_2$) by the atmospheric gases, *J. Chem. Phys.*, *71*, 3640-3647, 1979.

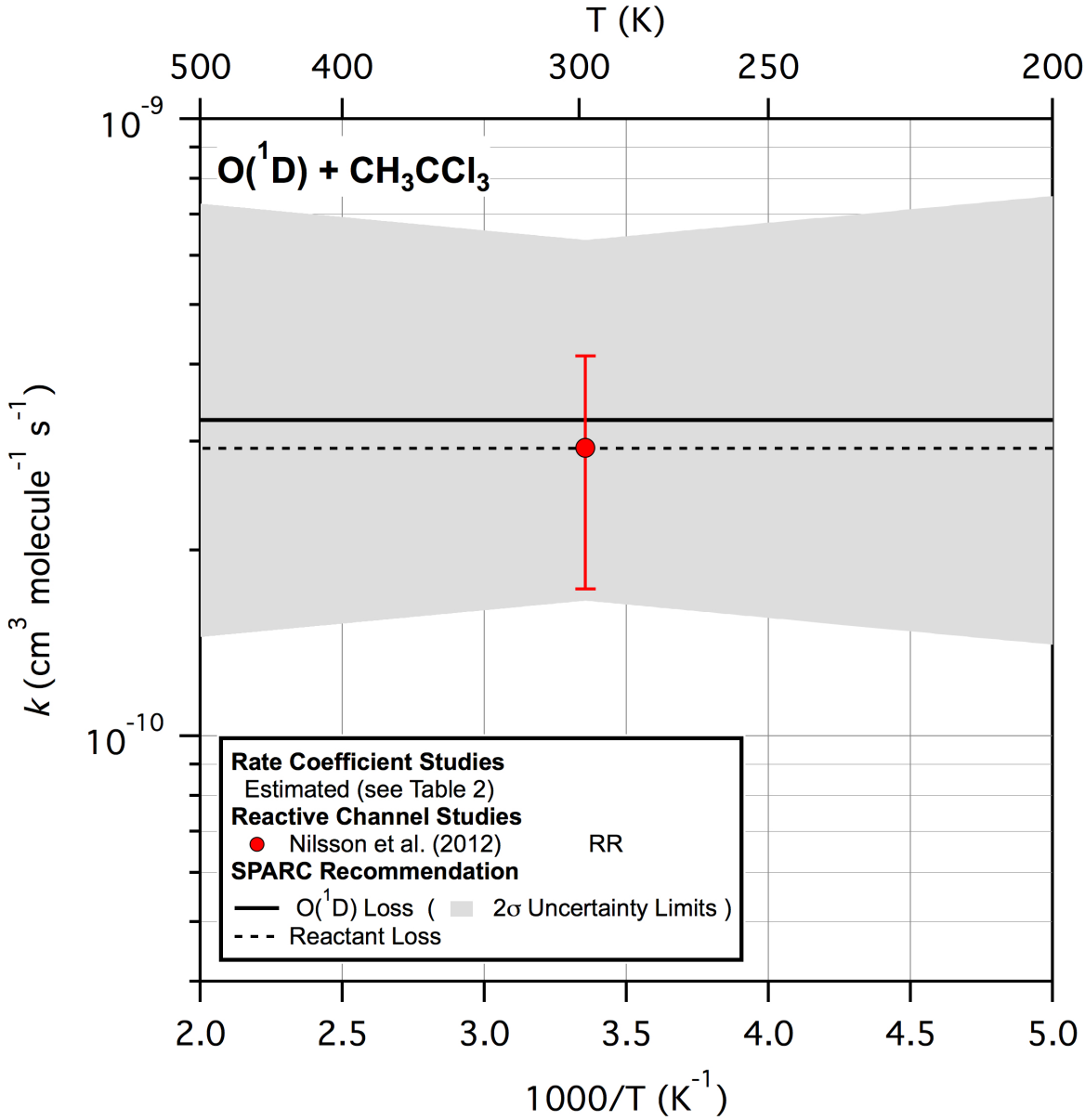
Blitz, M. A., T. J. Dillon, D. E. Heard, M. J. Pilling, and I. D. Trought, Laser induced fluorescence studies of the reactions of O(^{1}D$_2$) with N_2, O_2, N_2O, CH_4, H_2, CO_2, Ar, Kr and n-C_4H_{10}, *Phys. Chem. Chem. Phys.*, *6*, 2162-2171, 2004.

Davidson, J. A., H. I. Schiff, G. E. Streit, J. R. McAfee, A. L. Schmeltekopf, and C. J. Howard, Temperature dependence of O(^{1}D) rate constants for reactions with N_2O, H_2, CH_4, HCl, and NH_3, *J. Chem. Phys.*, *67,* 5021-5025, 1977.

Dillon, T. J., A. Horowitz, and J. N. Crowley, Absolute rate coefficients for the reactions of $O(^1D)$ with a series of n-alkanes, *Chem. Phys. Lett.*, *443*, 12-16, 2007.

Vranckx, S., J. Peeters, and S. Carl, A temperature dependence kinetic study of $O(^1D) + CH_4$: Overall rate coefficient and product yields, *Phys. Chem. Chem. Phys.*, *10*, 5714-5722, 2008.

13. CH_3CCl_3 (Methyl Chloroform)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 3.25 \times 10^{-10} \exp(0/T)$ cm^3 $molecule^{-1}$ s^{-1}

$k(298\ K) = 3.25 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.4$

$g = 0$

Recommended Reactive Yield: Reactant Loss

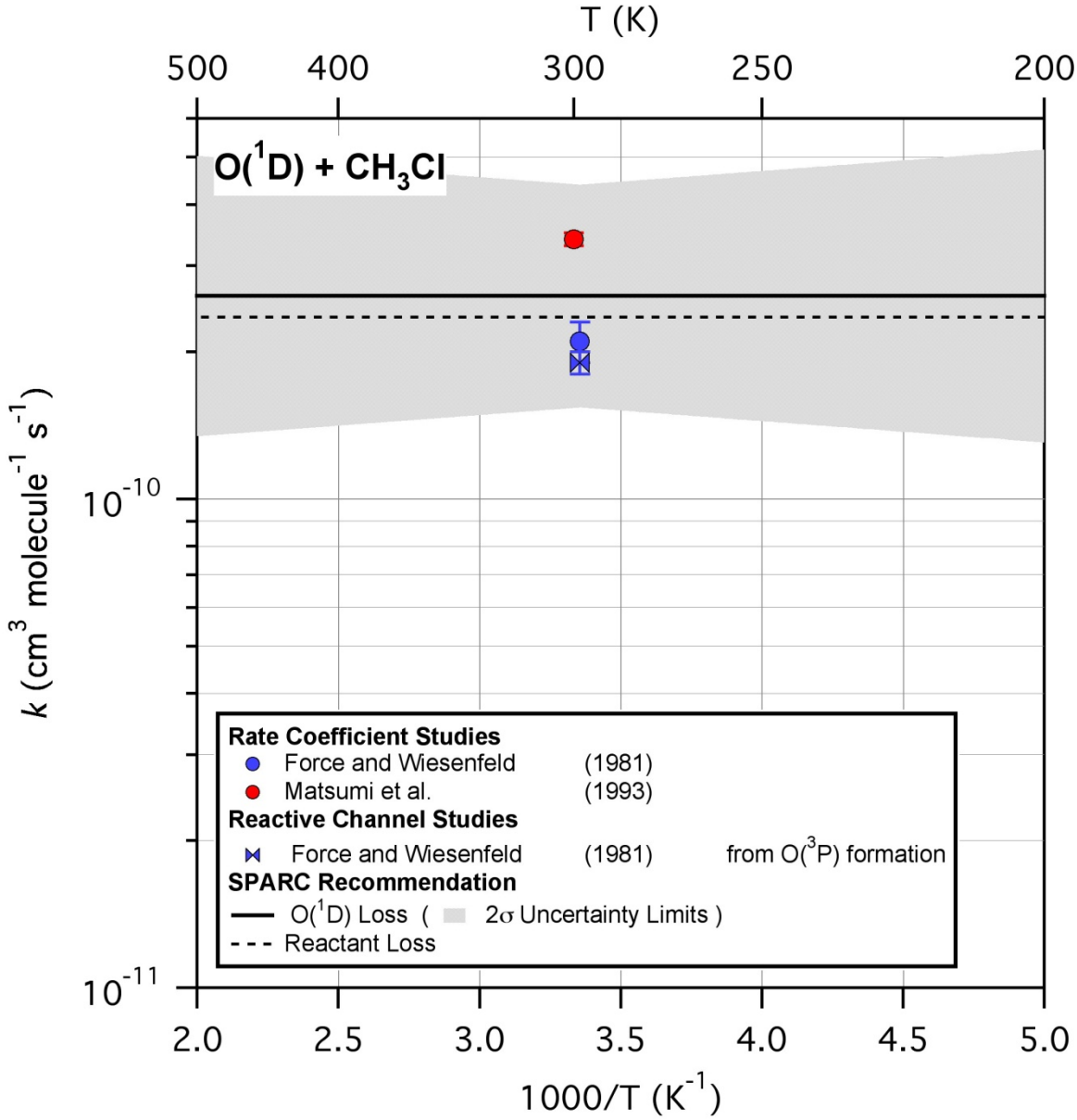
0.9 estimated

Not evaluated in JPL10-6

Reference

Nilsson, E. J. K., V. F. Andersen, O. J. Nielsen, and M. S. Johnson, Rate coefficients for the chemical reactions of CH_2F_2, $CHClF_2$, CH_2FCF_3 and CH_3CCl_3 with $O(^1D)$ at 298 K. *Chem. Phys. Lett.*, *554*, 27-32, 2012.

14. CH_3Cl (Methyl Chloride)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 2.6 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 2.6 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.3$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.905 ± 0.06

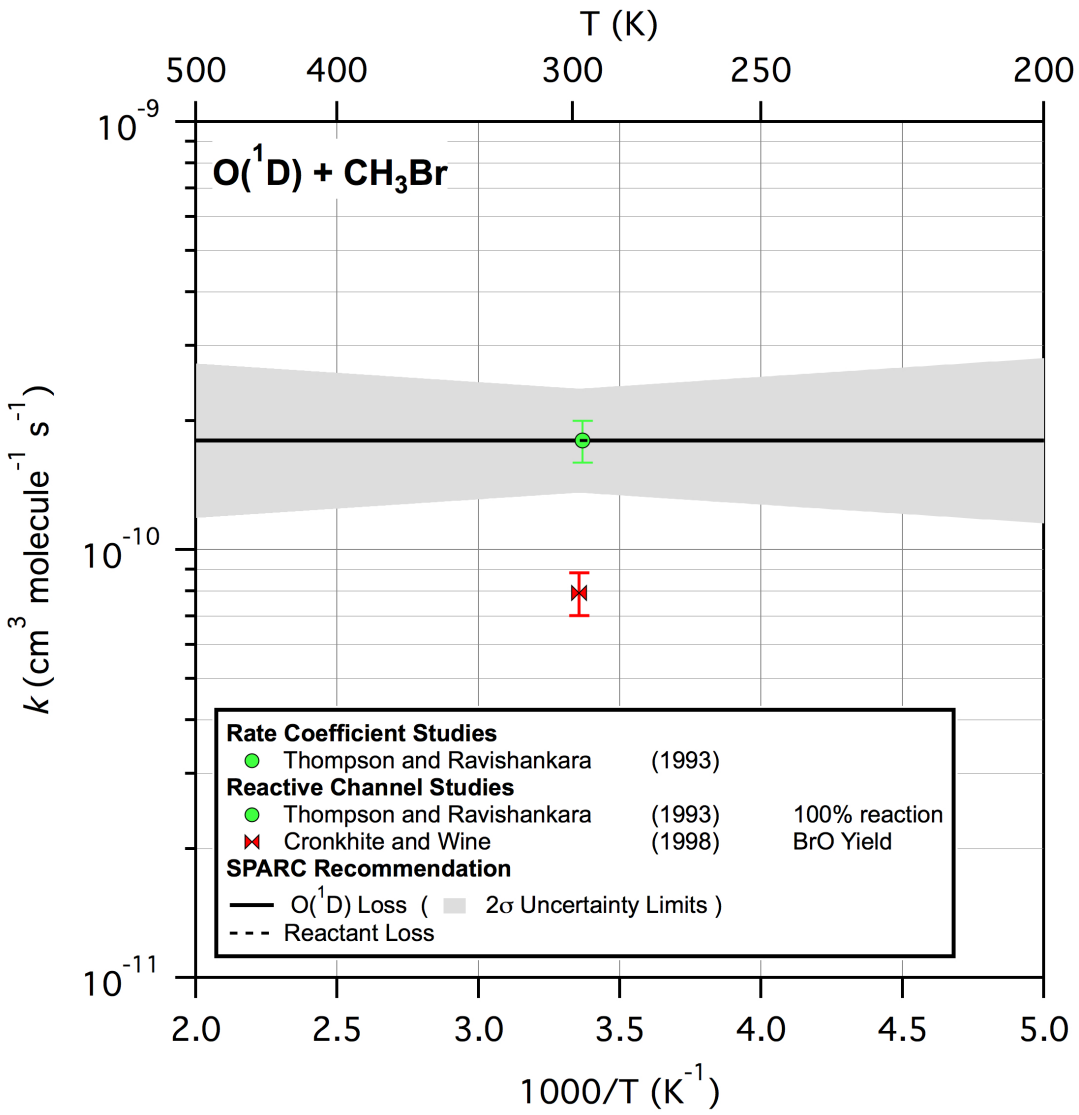
Not evaluated in JPL10-6

References

Force, A. P., and J. R. Wiesenfeld, Collisional deactivation of O(^{1}D$_2$) by the halomethanes. direct determination of reaction efficiency, *J. Phys. Chem.*, *85*, 782-785, 1981.

Matsumi, Y., K. Tonokura, Y. Inagaki, and M. Kawasaki, Isotopic branching ratios and translational energy release of H and D atoms in reaction of O(^{1}D) atoms with alkanes and alkyl chlorides, *J. Phys. Chem.*, *97*, 6816-6821, 1993.

15. CH_3Br (Methyl Bromide)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.8 \times 10^{-10} \exp(0/T)$ cm^3 $molecule^{-1}$ s^{-1}

$k(298\ K) = 1.8 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.15$

$g = 50$

Recommended Reactive Yield: Reactant Loss

1.0 +0/-0.07

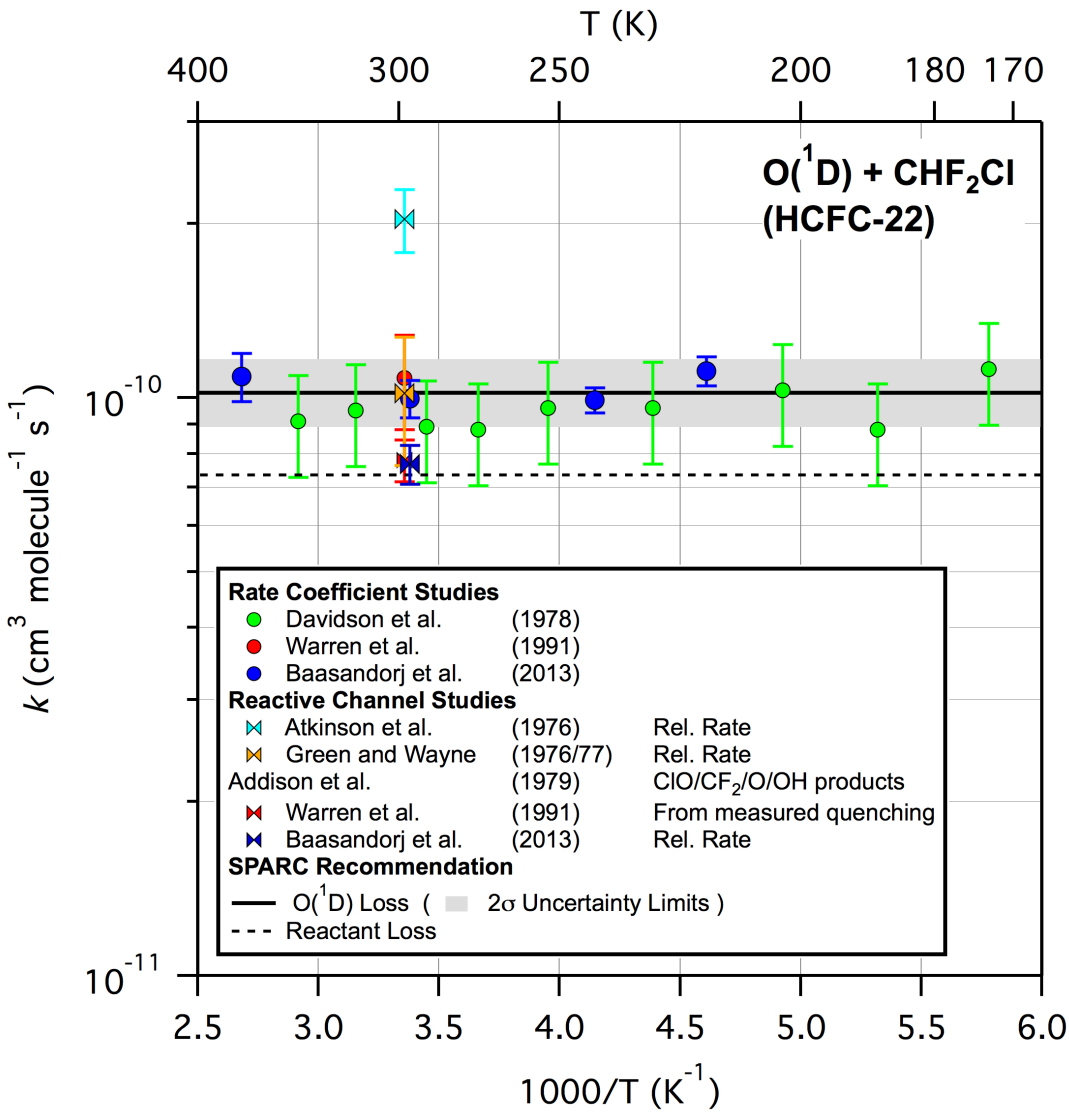
All parameters unchanged from JPL10-6

References

Cronkhite, J. M., and P. H. Wine, Branching ratios for BrO production from reactions of $O(^1D)$ with HBr, CF_3Br, CH_3Br, CF_2ClBr, and CF_2HBr, *Int. J. Chem. Kinet.*, *30,* 555-563, 1998.

Thompson, J. E., and A. R. Ravishankara, Kinetics of $O(^1D)$ reactions with bromocarbons, *Int. J. Chem. Kinet.*, *25*, 479-487, 1993.

16. CHF_2Cl (HCFC-22)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.02 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.02 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.07$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.72 ± 0.06

Revised from JPL10-6

References

Addison, M. C., R. J. Donovan, and J. Garraway, Reactions of $O(^1D)$ and $O(^3P)$ with halogenomethanes, *Faraday Disc. Chem. Soc., 67*, 286-296, 1979.

Atkinson, R., G. M. Breuer, J. N. Pitts, Jr., and H. L. Sandoval, Tropospheric and stratospheric sinks for halocarbons: Photooxidation, $O(^1D)$ atom, and OH radical reactions, *J. Geophys. Res., 81*, 5765-5770, 1976.

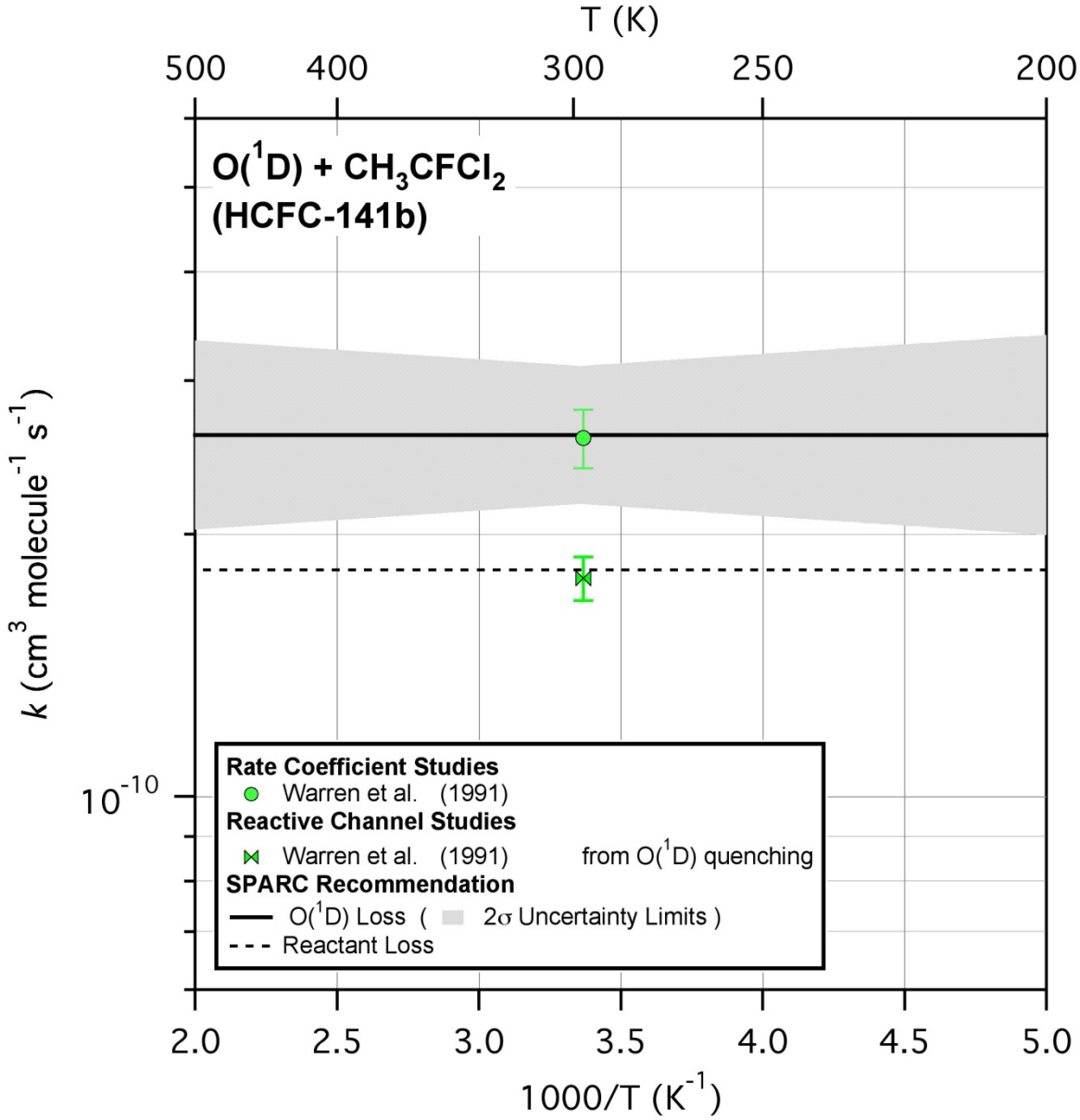
Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, $O(^1D)$ kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Davidson, J. A., H. I. Schiff, T. J. Brown, and C. J. Howard, Temperature dependence of the rate constants for reactions of $O(^1D)$ atoms with a number of halocarbons, *J. Chem. Phys.*, *69*, 4277-4279, 1978.

Green, R. G., and R. P. Wayne, Relative rate constants for the reactions of $O(^1D)$ atoms with fluorochlorocarbons and with N_2O, *J. Photochem.*, *6*, 371-374, 1976/77.

Warren, R., T. Gierczak, and A. R. Ravishankara, A study of $O(^1D)$ reactions with CFC substitutes, *Chem. Phys. Lett., 183*, 403-409, 1991.

17. CH_3CFCl_2 (HCFC-141b)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 2.6 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 2.6 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

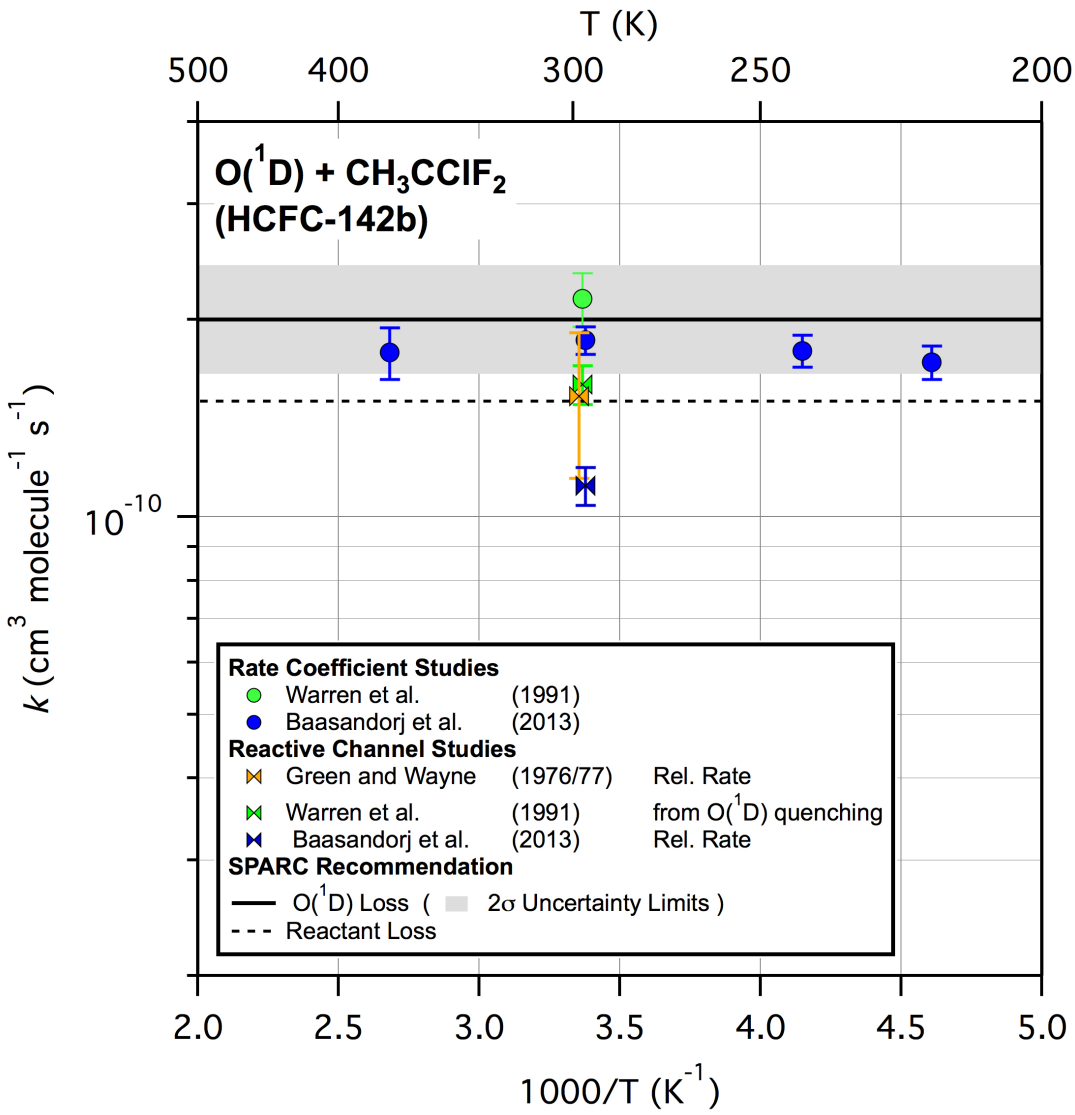
0.70 ± 0.05

All parameters unchanged from JPL10-6

Reference

Warren, R., T. Gierczak, and A. R. Ravishankara, A study of O(^{1}D) reactions with CFC substitutes, *Chem. Phys. Lett., 183*, 403-409, 1991.

18. CH_3CF_2Cl (HCFC-142b)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 2.0 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 2.0 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.1$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.75 ± 0.05

Revised from JPL10-6

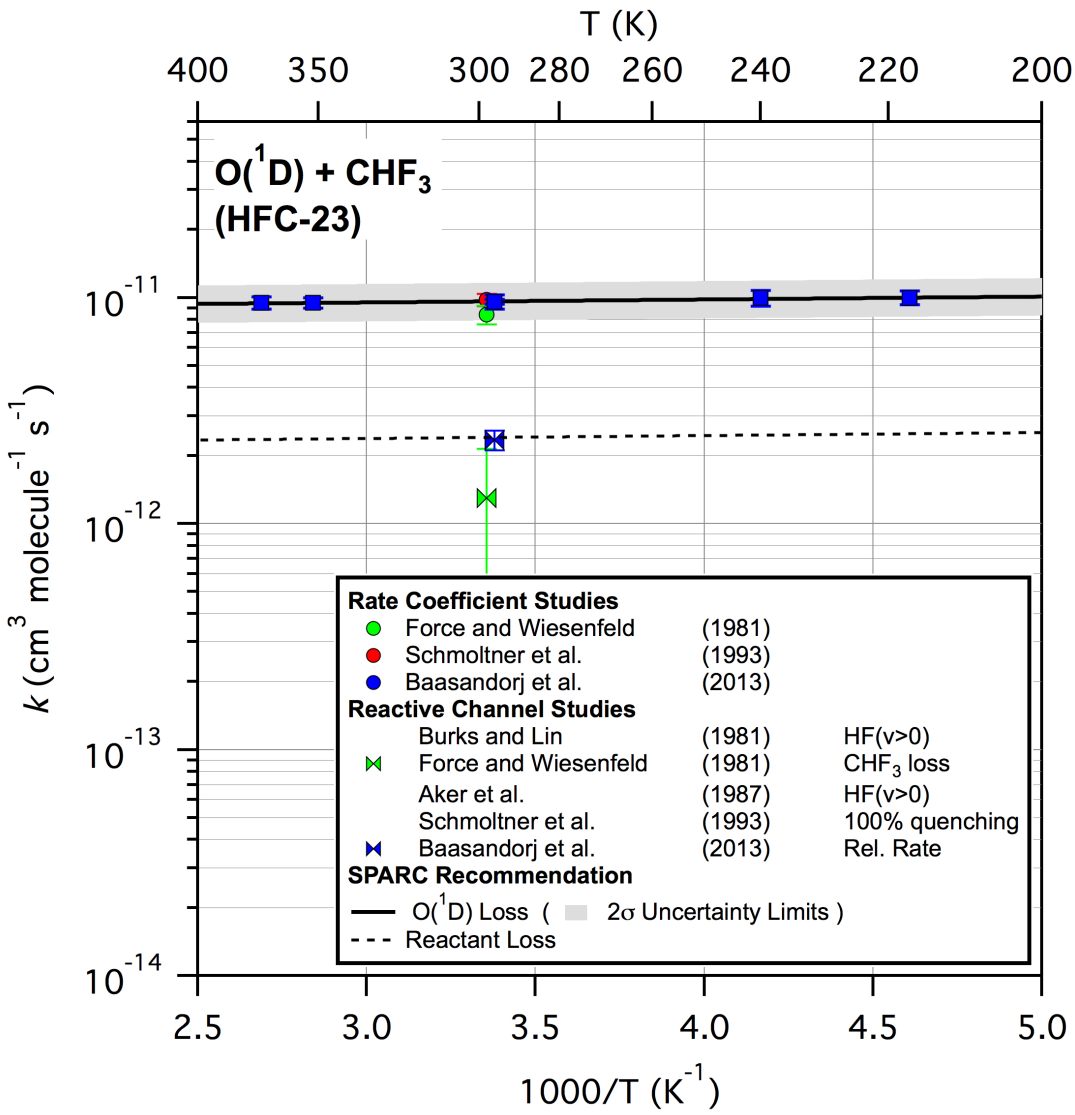
References

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, $O(^1D)$ kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Green, R. G., and R. P. Wayne, Relative rate constants for the reactions of $O(^1D)$ atoms with fluorochlorocarbons and with N_2O, *J. Photochem.*, *6*, 371-374, 1976/77.

Warren, R., T. Gierczak, and A. R. Ravishankara, A study of $O(^1D)$ reactions with CFC substitutes, *Chem. Phys. Lett., 183*, 403-409, 1991.

19. CHF_3 (HFC-23)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 8.7 \times 10^{-12} \exp(30/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 8.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.05$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.25 ± 0.05

Revised from JPL10-6

References

Aker, P. M., B. I. Niefer, J. J. Sloan, and H. Heydtmann, The dynamics and microscopic kinetics of the reactions of O(^{1}D$_2$) atoms with $CHCl_3$ and CHF_3, *J. Chem. Phys.*, 87, 203-209, 1987.

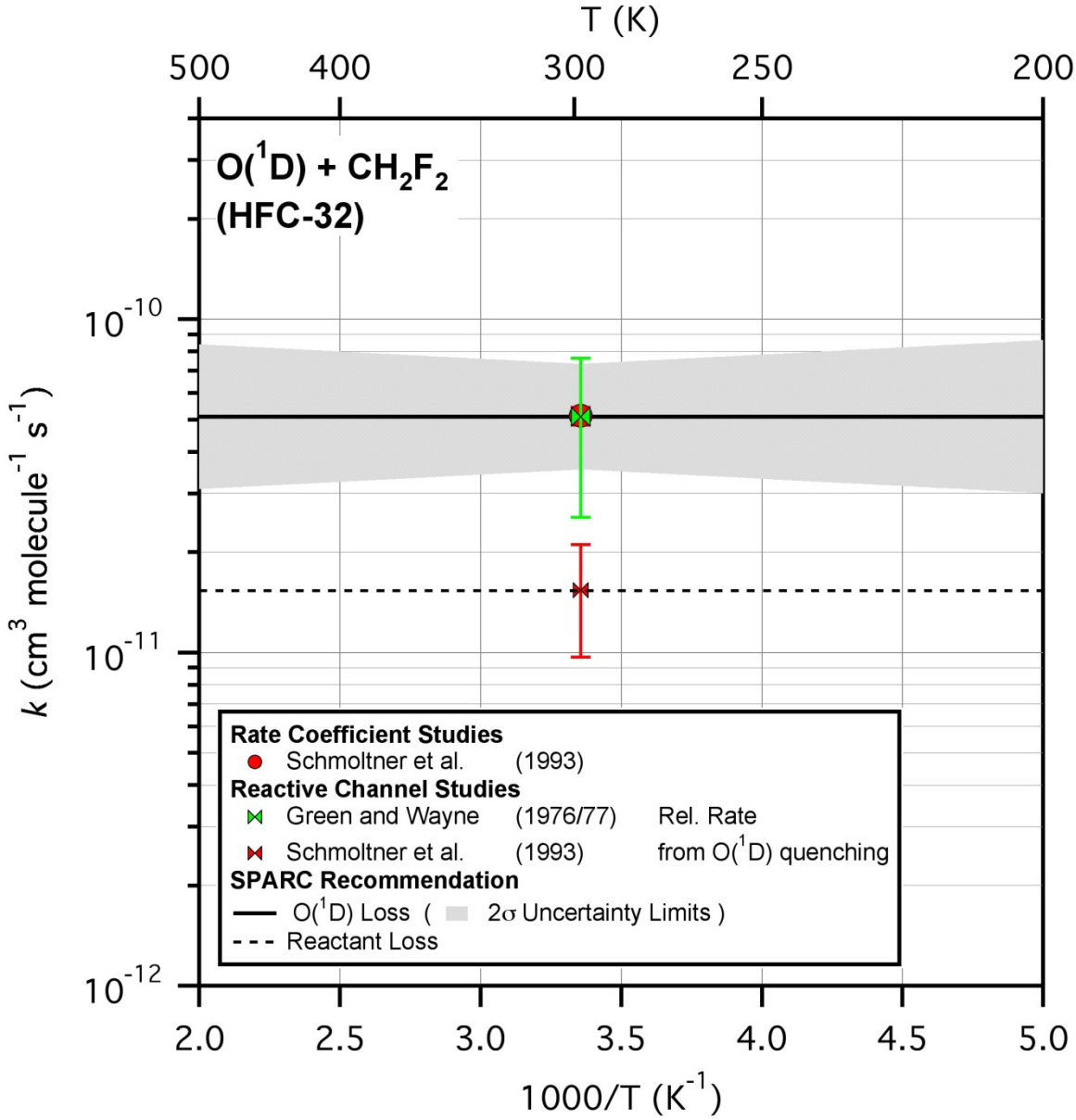
Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, O(^{1}D) kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Burks, T. L., and M. C. Lin, The dynamics of formation of vibrationally excited HF in reactions of $O(2^1D_2)$ atoms with partially fluorinated alkanes, *Int. J. Chem. Kinet.*, *13*, 977-999, 1981.

Force, A. P., and J. R. Wiesenfeld, Collisional Deactivation of $O(^1D_2)$ by the Halomethanes. Direct Determination of Reaction Efficiency, *J. Phys. Chem.*, *85*, 782-785, 1981.

Schmoltner, A.-M., R. K. Talukdar, R. F. Warren, A. Mellouki, L. Goldfarb, T. Gierczak, S. A. McKeen, and A. R. Ravishankara, *J. Phys. Chem.*, *97*, 8976-8982, 1993.

20. CH_2F_2 (HFC-32)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 5.1 \times 10^{-11} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\text{ K}) = 5.1 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\text{ K}) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.30 ± 0.10

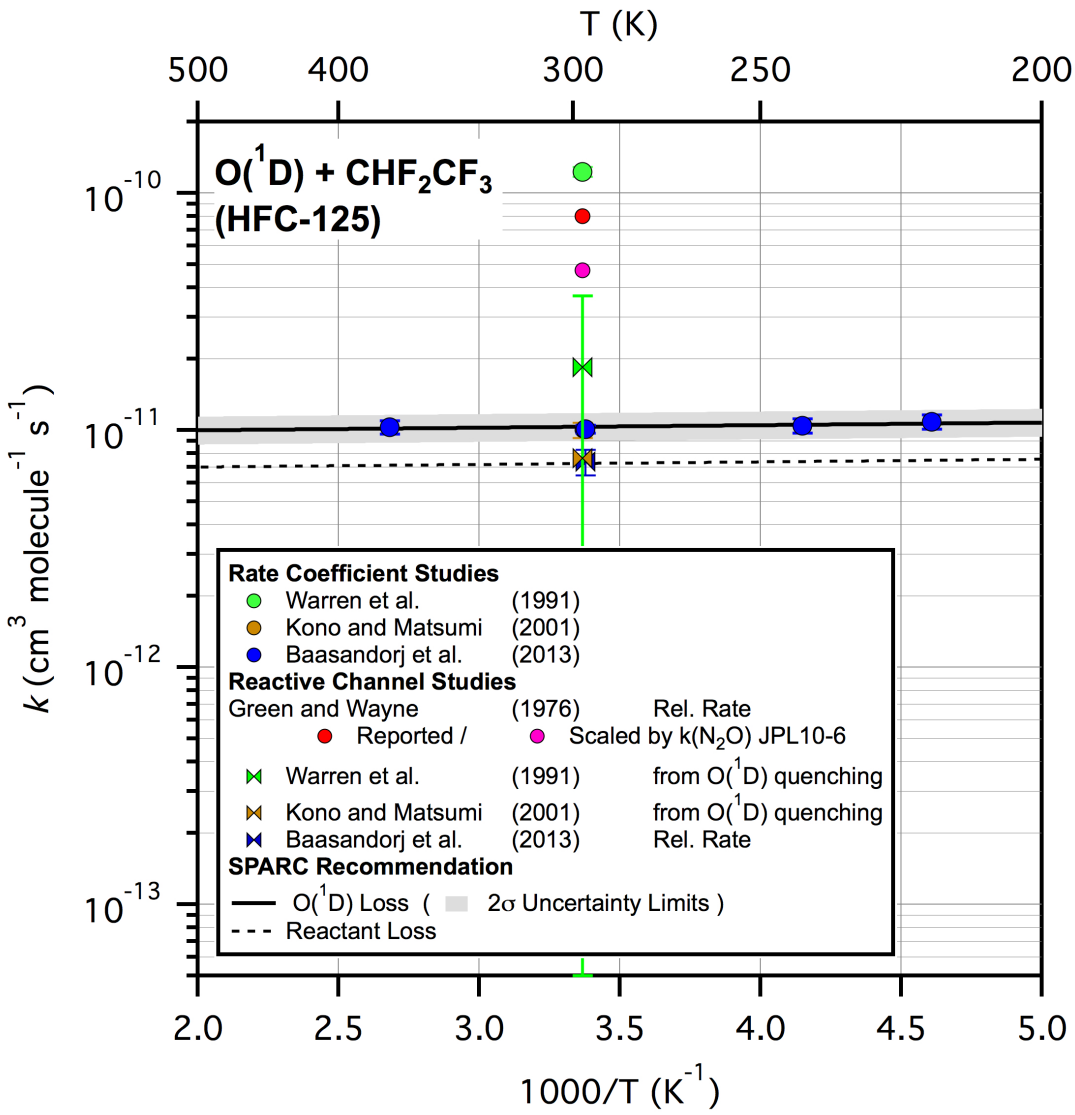
All parameters unchanged from JPL10-6

References

Green, R. G., and R. P. Wayne, Relative rate constants for the reactions of O(^{1}D) atoms with fluorochlorocarbons and with N_2O, *J. Photochem.*, *6*, 371-374, 1976/77.

Schmoltner, A.-M., R. K. Talukdar, R. F. Warren, A. Mellouki, L. Goldfarb, T. Gierczak, S. A. McKeen, and A. R. Ravishankara, *J. Phys. Chem.*, *97*, 8976-8982, 1993.

21. CHF_2CF_3 (HFC-125)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 9.5 \times 10^{-12} \exp(25/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.05 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.07$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.70 ± 0.09

Revised from JPL10-6

References

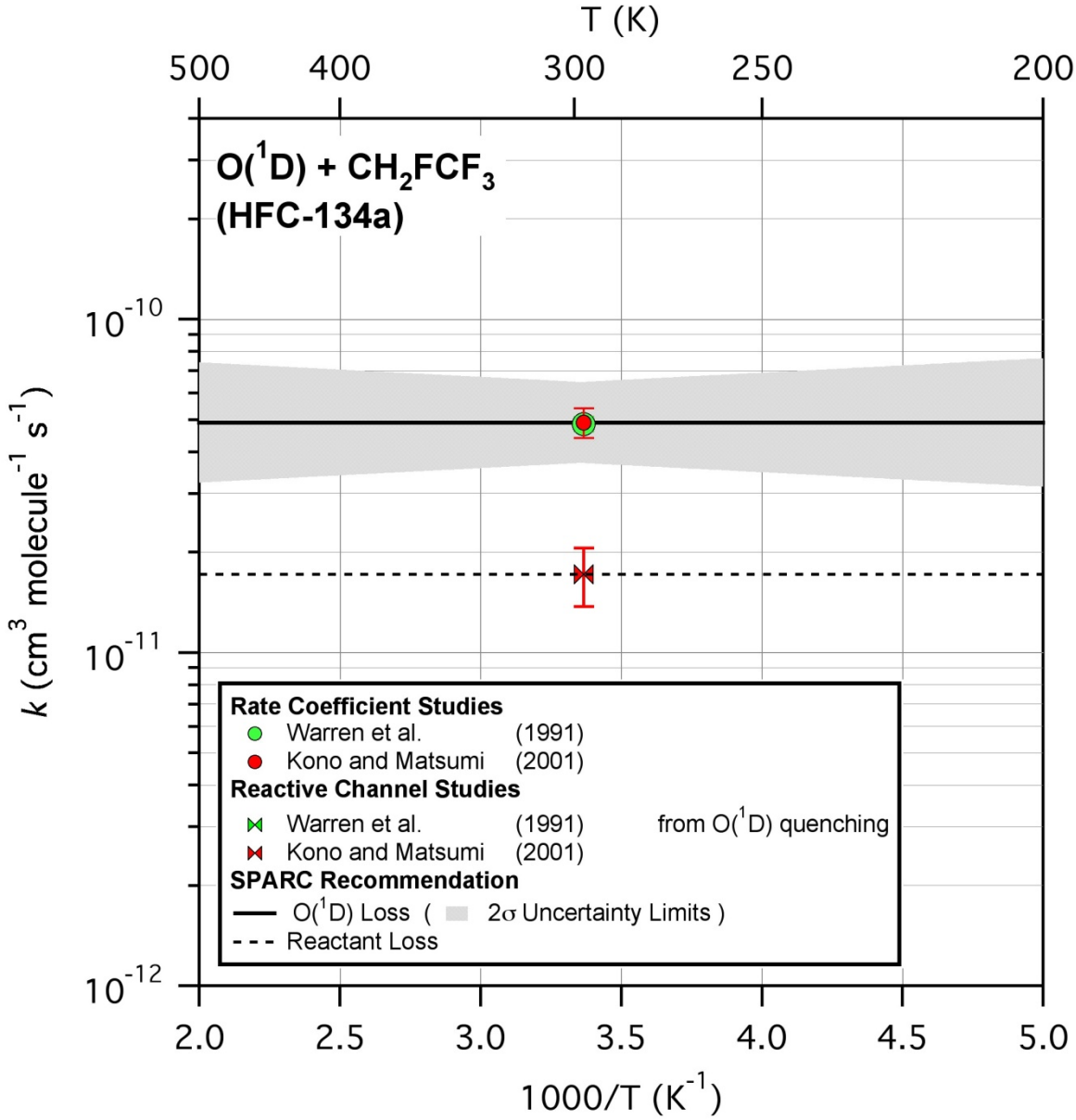
Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, $O(^1D)$ kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Green, R. G., and R. P. Wayne, Relative rate constants for the reactions of $O(^1D)$ atoms with fluorochlorocarbons and with N_2O, *J. Photochem.*, *6*, 371-374, 1976/77.

Kono, M., and Y. Matsumi, Reaction processes of $O(^1D)$ with fluoroethane compounds, *J. Phys. Chem.*, *105*, 65 -69, 2001.

Warren, R., T. Gierczak, and A. R. Ravishankara, A study of $O(^1D)$ reactions with CFC substitutes, *Chem. Phys. Lett., 183*, 403-409, 1991.

22. CH_2FCF_3 (HFC-134a)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 4.9 \times 10^{-11} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 4.9 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.15$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.35 ± 0.06

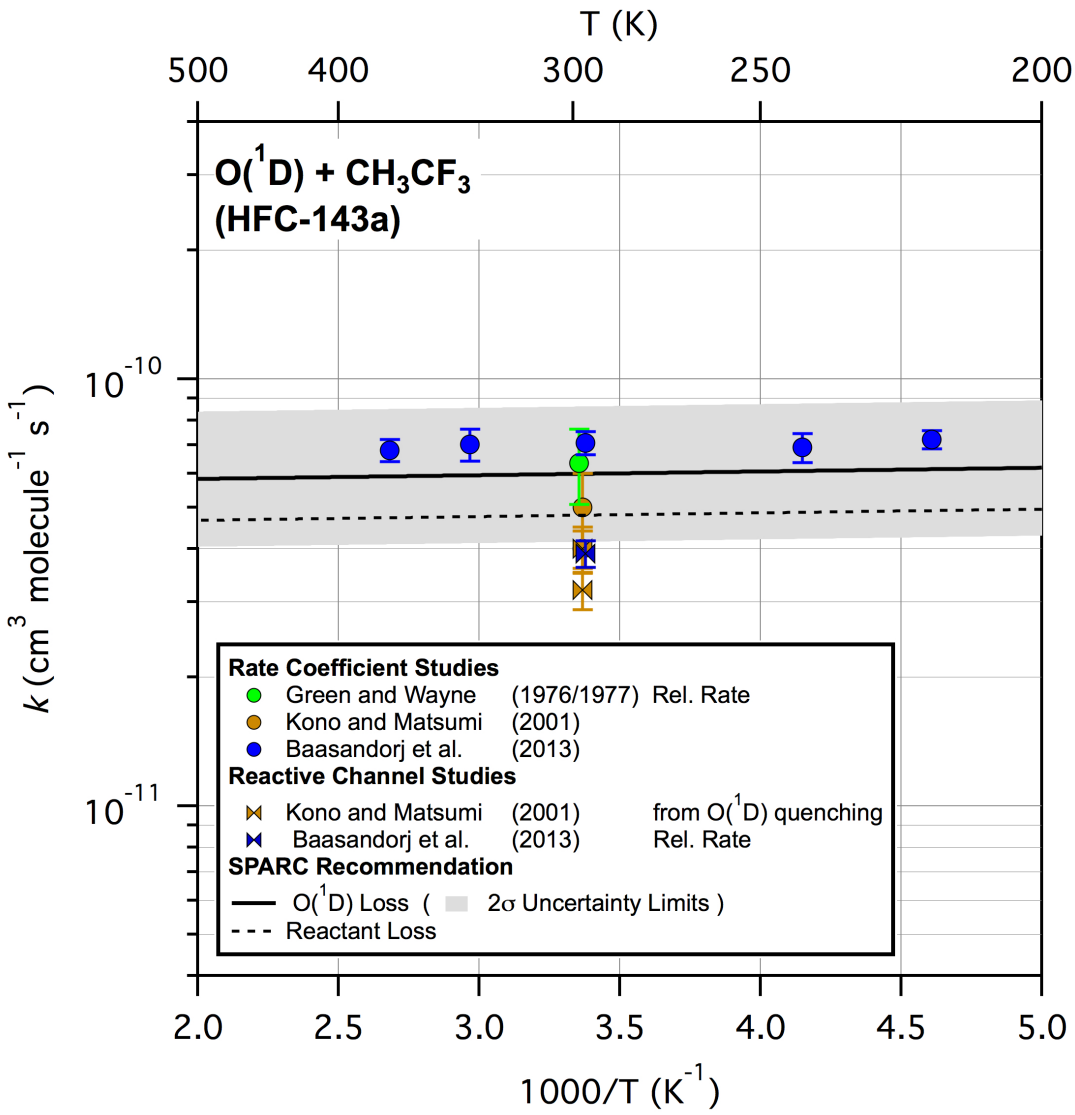
All parameters unchanged from JPL10-6

References

Kono, M., and Y. Matsumi, Reaction processes of O(^{1}D) with fluoroethane compounds, *J. Phys. Chem.*, *105*, 65-69, 2001.

Warren, R., T. Gierczak, and A. R. Ravishankara, A study of O(^{1}D) reactions with CFC substitutes, *Chem. Phys. Lett., 183*, 403-409, 1991.

23. CH_3CF_3 (HFC-143a)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 5.6 \times 10^{-11} \exp(20/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 6.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.2$

$g = 0$

Revised from JPL10-6

Recommended Reactive Yield: Reactant Loss

0.80 ± 0.20

Revised from JPL10-6

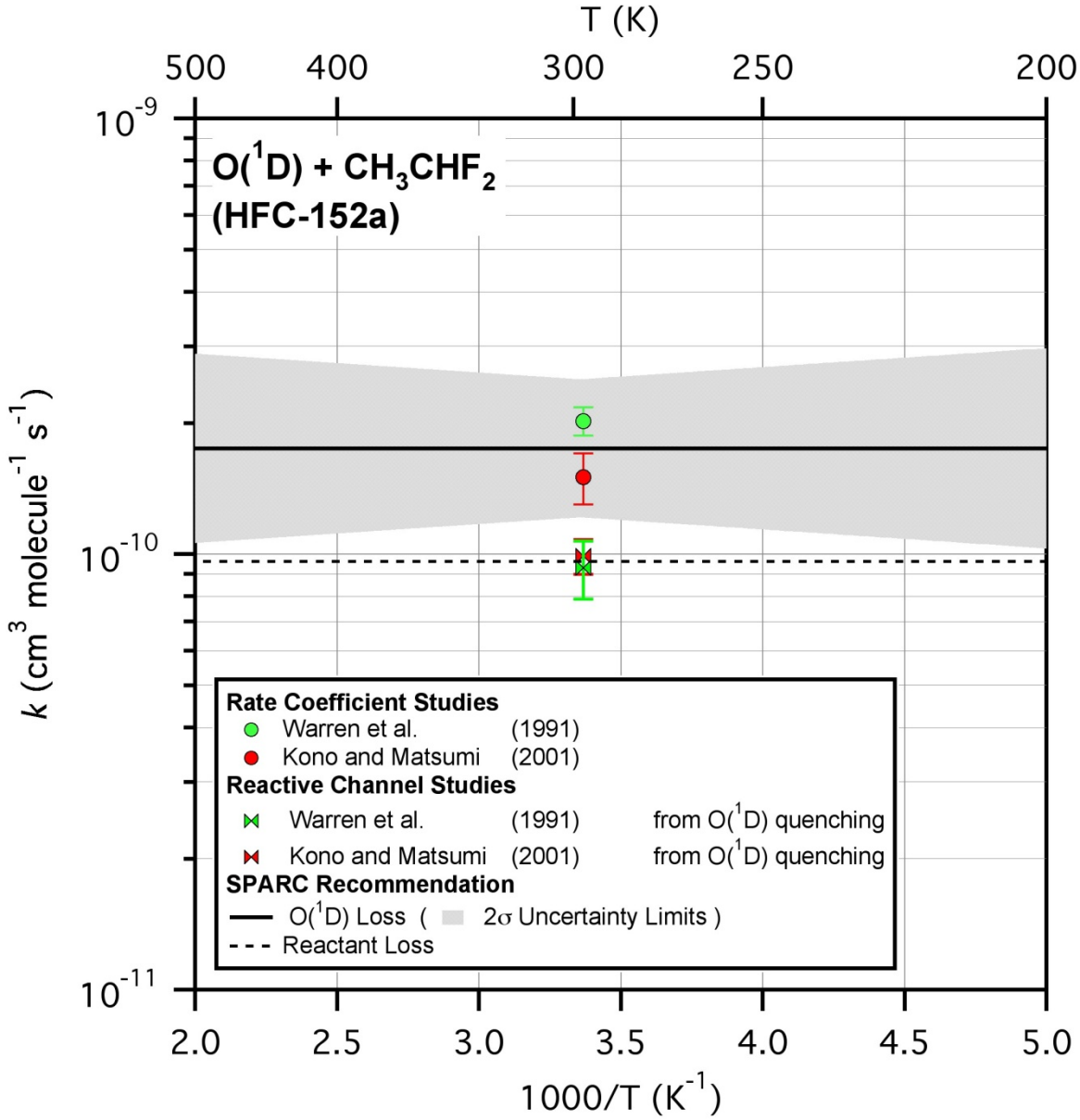
References

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, O(^{1}D) kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

Green, R. G., and R. P. Wayne, Relative rate constants for the reactions of O(^{1}D) atoms with fluorochlorocarbons and with N_2O, *J. Photochem.*, *6*, 371-374, 1976/77.

Kono, M., and Y. Matsumi, Reaction processes of O(^{1}D) with fluoroethane compounds, *J. Phys. Chem.*, *105*, 65-69, 2001.

24. CH_3CHF_2 (HFC-152a)



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 1.75 \times 10^{-10} \exp(0/T)$ cm^3 $molecule^{-1}$ s^{-1}

$k(298\ K) = 1.75 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.2$

$g = 50$

Recommended Reactive Yield: Reactant Loss

0.55 ± 0.20

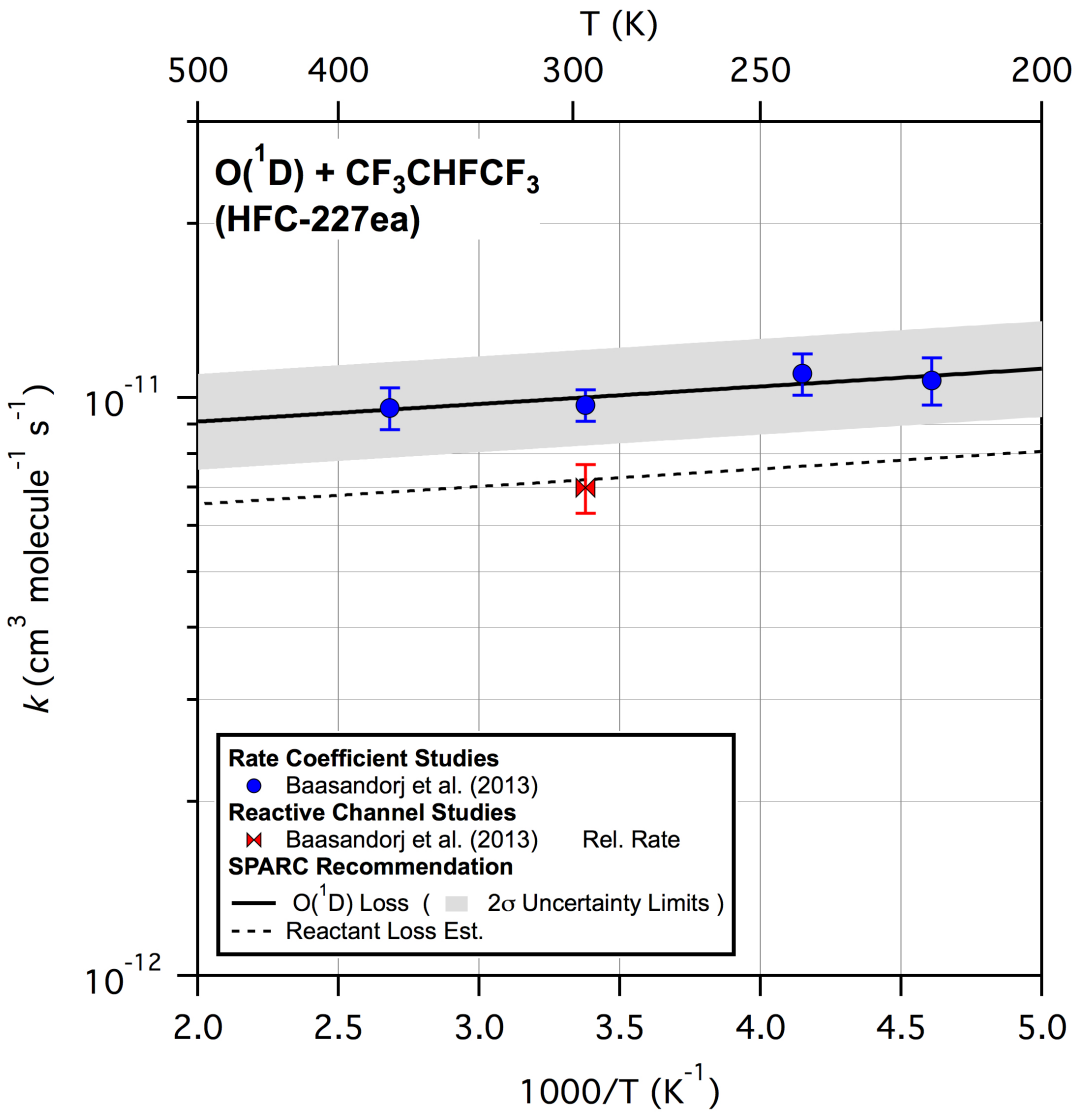
All parameters unchanged from JPL10-6

References

Kono, M., and Y. Matsumi, Reaction processes of $O(^1D)$ with fluoroethane compounds, *J. Phys. Chem.*, *105*, 65-69, 2001.

Warren, R., T. Gierczak, and A. R. Ravishankara, A study of $O(^1D)$ reactions with CFC substitutes, *Chem. Phys. Lett., 183*, 403-409, 1991.

25. CF_3CHFCF_3 (HFC-227ea)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 7.9 \times 10^{-12} \exp(70/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.1$

$g = 0$

Recommended Reactive Yield: Reactant Loss

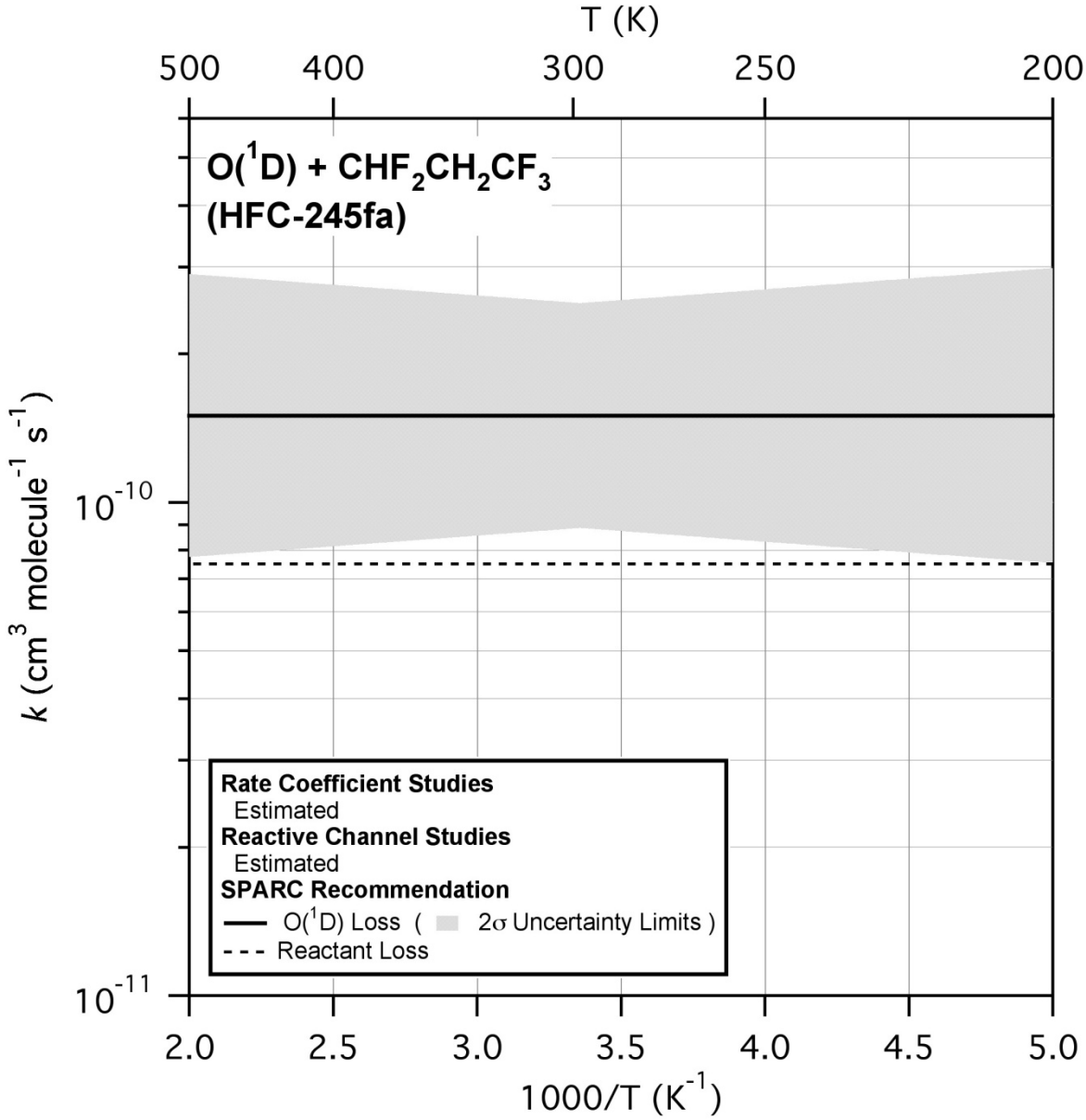
0.72 ± 0.07

Not evaluated in JPL10-6

Reference

Baasandorj, M., E. L. Fleming, C. H. Jackman, and J. B. Burkholder, O(^{1}D) kinetic study of key ozone depleting substances and greenhouse gases, *J. Phys. Chem. A*, dx.doi.org/10.1021/jp310910f, 2013.

26. $CHF_2CH_2CF_3$ (HFC-245fa)



Recommended Rate Coefficient: O(^{1}D) Loss

$k(T) = 1.5 \times 10^{-10} \exp(0/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 1.5 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Recommended Uncertainty Factors

$f(298\ K) = 1.3$

$g = 0$

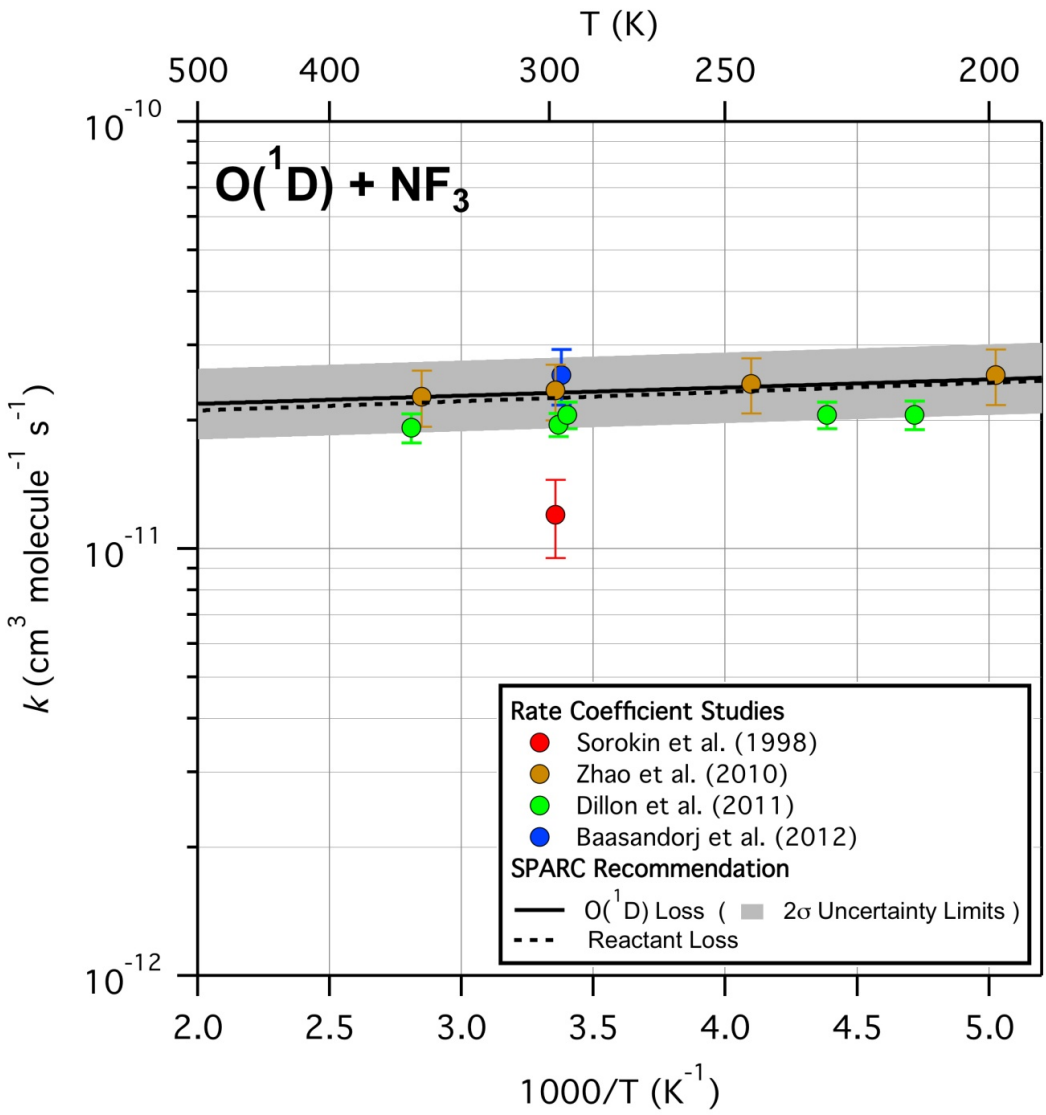
Recommended Reactive Yield: Reactant Loss

0.5

Parameters estimated

Not evaluated in JPL10-6

27. NF_3



Recommended Rate Coefficient: $O(^1D)$ Loss

$k(T) = 2.0 \times 10^{-11} \exp(44/T)$ cm^3 molecule^{-1} s^{-1}

$k(298\ K) = 2.3 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}

Revised from JPL 10-6

Recommended Uncertainty Factors

$f(298\ K) = 1.1$

$g = 0$

Recommended Reactive Yield: Reactant Loss

0.93 (+0.07/-0.21)

Revised from JPL 10-6

References

Baasandorj, M., B. D. Hall, and J. B. Burkholder, Rate coefficients for the reaction of $O(^1D)$ with the atmospherically long-lived greenhouse gases NF_3, SF_5CF_3, CHF_3, C_2F_6, c-C_4F_8, n-C_5F_{12}, and n-C_6F_{14}, *Atmos. Chem. Phys.*, *12*, 11753-11764, 2012.

Dillon, T. J., L. Vereecken, A. Horowitz, V. Khamaganov, J. N. Crowley, and J. Lelieveld, Removal of the potent greenhouse gas NF_3 by reactions with the atmospheric oxidants $O(^1D)$, OH and O_3, *Phys. Chem. Chem. Phys.*, *13*, 18600-18608, 2011.

Sorokin, V. I., N. P. Gristan, and A. I. Chichinin, Collisions of $O(^1D)$ with HF, F_2, XeF_2, NF_3, and CF_4: Deactivation and reaction, *J. Chem. Phys.*, *108*, 8995-9003, 1998.

Zhao, Z., P. L. Laine, J. M. Nicovich, and P. H. Wine, Reactive and non-reactive quenching of $O(^1D)$ by the potent greenhouse gases SO_2F_2, NF_3, and SF_5CF_3, *Proc. Nat. Acd. Sci.*, *107*, 6610-6615, 2010.