Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheets for Halogenated Oxy Radical Decomposition; oFOx45 – oFOx54 and oRClOx1 – oRClOx33.

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$$R_1(R_2)CHO + O_2 \rightarrow R_1COR_2 + HO_2 \text{ (or} \rightarrow \text{products)} \qquad (1)$$

$$R_1(R_2)CHO \text{ (+ M)} \rightarrow \text{ products} \qquad (2)$$

R = alkyl, halogenated alkyl, H or halogen atom

Rate coefficient data

Reactions		k_1/k_2 /cm^2 molecule^{-1}	Temp/K	Reference	Comments
$CH_2FO + O_2 \rightarrow HCOF + HO_2$	(1)	$k_1[O_2] \gg k_2$ (933 mbar,air)	298	Edney and Driscoll, 1992	(a)
$CH_2FO + M \rightarrow HCOF + H + M$	(2)	$k_1[O_2] \gg k_2$ (986 mbar,air)	298	Tuazon and Atkinson, 1993	(a)
$CH_3CF_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (933 mbar,air)	298	Edney and Driscoll, 1992	(b)
$CH_3CF_2O + M \rightarrow CH_3 + COF_2 + M$	(2)	$k_1[O_2] \ll k_2$ (986 mbar,air)	298	Tuazon and Atkinson, 1993	(c)
$CH_2FCHFO + O_2 \rightarrow CH_2FCOF + HO_2$	(1)	$k_1[O_2] \gg k_2$ (933 mbar,air)	296	Wallington et al., 1994	(d)
$CH_2FCHFO + M \rightarrow CH_2F + HCOF + M$	(2)				
$CF_3CHFO + O_2 \rightarrow CF_3COF + HO_2$	(1)	$1.58 \times 10^{-25} \exp(3600/T)$	261-353	Wallington et al., 1992	(e)
$CF_3CHFO + M \rightarrow CF_3 + HCOF + M$	(2)	2.8×10^{-20} (2 atm)	298		
		$3.2 \times 10^{-25} \exp(3510/T)$	273-320	Tuazon and Atkinson, 1993	(f)
		4.5×10^{-20} (986 mbar)	298		
		$k_2 = 3.7 \times 10^7 \exp(-2200/T) s^{-1}$	211-372	Maricq and Szente, 1992	(g)
		$k_2 = 2.3 \times 10^4 s^{-1}$ (306mbar)	298		
		$1.18 \times 10^{-24} \exp(2860/T)$	235-318	Rattigan et al., 1994	(h)
		1.7×10^{-20} (1 bar)	298		
		1.5×10^{-19} (50 mbar)	300	Bednarek et al, 1996	(i)
		$k_1 = 2.7 \times 10^{-15}$	300		
		$8.7 \times 10^{-25} \exp(3240/T)$ (1 bar)	244-295		
		$2.1 \times 10^{-25} \exp(3625/T)$ (1 bar)	238-295	Wallington et al, 1996	(j)

		1.38×10^{-24} exp(2400/T) (1 bar)	298-357	Hasson et al., 1998	(k)
$CF_3CF_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (933 mbar,air)	298	Tuazon and Atkinson, 1993	(e)
$CF_3CF_2O + M \rightarrow CF_3 + CF_2O + M$	(2)				
$CH_3CF_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (933 mbar, air)	298	Edney and Driscoll, 1992	(l)
$CH_3CF_2O + M \rightarrow CH_3 + COF_2 + M$	(2)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1993	(m)
$CHFClO + O_2 \rightarrow COFCl + HO_2$	(1)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1993	(n)
$CHFClO + M \rightarrow HCOF + Cl + M$	(2)				
$CF_2ClO + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (933 mbar, air)	298	Edney and Driscoll, 1992	(o)
$CF_2ClO + M \rightarrow COF_2 + Cl + M$	(2)	$k_2 = 7.0 \times 10^5$	298	Carr et al.,(1986); Rayez et al. (1987)	FP-UVA
		$k_2 = 3 \times 10^{13}$exp(-5250/T) (k/s^{-1})			
$CFCl_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1993	(p)
$CFCl_2O + M \rightarrow COFCl + Cl + M$	(2)	$k_2 = 7.0 \times 10^5$		Lesclaux et al. (1987); Rayez et al. (1987)	FP-MS
		$k_2 = 3 \times 10^{13}$exp(-5250/T) (k/s^{-1})			
$CCl_3O + M \rightarrow COCl_2 + Cl + M$	(2)	$k_2 = 8.0 \times 10^6$		Lesclaux et al. (1987); Rayez et al. (1987)	FP-MS (p)
		$k_2 = 4 \times 10^{13}$exp(-4600/T) (k/s^{-1})			
$CF_2ClCH_2O + O_2 \rightarrow CF_2ClCHO + HO_2$	(1)	$k_1[O_2] \gg k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1994	(q)
$CF_2ClCH_2O + M \rightarrow CF_2Cl + HCHO + M$	(2)				
$CFCl_2CH_2O + O_2 \rightarrow CFCl_2CHO + HO_2$	(1)	$k_1[O_2] \gg k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1994	(r)
$CFCl_2CH_2O + M \rightarrow CFCl_2 + HCHO + M$	(2)				
		$k_1 = 2.0 \times 10^{-15}$	298	Mörs et al, 1996	(s)
		$k_1 = 1.3 \times 10^{-16}$	298	Wu and Carr, 1996	(t)
		$k_1 = 2.4 \times 10^{-15}$exp[-(944 ± 55)/T]	251-341		
$CF_3CFClO + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (933 mbar, air)	298	Edney and Driscoll, 1992	(u)
$CF_3CFClO + M \rightarrow CF_3COF + Cl + M$	(2)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1993	(v)
$CF_3CCl_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (933 mbar, air)	298	Edney et al., 1991	(w)
$CF_3CCl_2O + M \rightarrow CF_3COCl + Cl + M$	(2)	$k_1[O_2] \ll k_2$ (135 mbar, O_2)	298	Sato and Nakamura, 1991	(x)
		$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1993	(y)
		$k_1[O_2] \ll k_2$ (~ 1 bar, air)	298	Hayman et al., 1994	(z)

$CF_3CF_2CCl_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$ (135 mbar, O_2)	298	Sato and Nakamura, 1991	(aa)
$CF_3CF_2CCl_2O+M \rightarrow CF_3CF_2COCl+Cl+M$	(2)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1994	(bb)
$CF_2ClCF_2CFClO + O_2 \rightarrow$ products (1)	(1)	$k_1[O_2] \ll k_2$ (135 mbar, O_2)	298	Sato and Nakamura, 1991	(cc)
$CF_2ClCF_2CFClO+M \rightarrow CF_2ClCF_2COF+ Cl+M$	(2)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1994	(dd)
$CH_2ClO + O_2 \rightarrow HCOCl + HO_2$	(1)	4.6×10^{-18} (933 mbar, $O_2 + N_2$)	296	Kaiser and Wallington, 1993	(ee)
$CH_2ClO + M \rightarrow HCO + HCl + M$	(2)	$k_1 = 1.3 \times 10^{-12}\exp[-(934\pm128]/T)$ $k_2 = 7.7 \times 10^{9}\exp[-(4803\pm722]/T)$ (13 mbar)	265-306 265-306	Wu and Carr, 2001	(ff)
$CH_3CHClO + O_2 \rightarrow CH_3COCl + HO_2$	(1)	$k_1[O_2] \ll k_2$ (933 mbar, air)	295	Shi et al., 1993	(gg)
$CH_3CHClO + M \rightarrow CH_3CO + HCl + M$	(2)	$k_1[O_2] \ll k_2$ (1013 mbar, air)	298	Maricq et al., 1993	(hh)
$HOCH_2CHClO+O_2 \rightarrow HOCH_2COCl+HCl+HO_2$	(1)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1994	(ii)
$HOCH_2CHClO+M \rightarrow CH_2OH+HCOCl+M$	(2)				
$HOCHClCH_2O+O_2 \rightarrow HOCHClCHO+HO_2$	(1)	$k_1[O_2] \ll k_2$ (986 mbar, air)	298	Tuazon and Atkinson, 1994	(jj)
$HOCHClCH_2O+M \rightarrow CHClOH+HCHO+M$	(2)				
$CH_3CCl_2O + O_2 \rightarrow$ products (1)	(1)	$k_1[O_2] \ll k_2$ (933 mbar, O_2)	298	Nelson et al., 1990	(kk)
$CH_3CCl_2O + M \rightarrow CH_3COCl + Cl + M$	(2)				
$CCl_3CH_2O + O_2 \rightarrow CCl_3CHO + HO_2$	(1)	$k_1[O_2] \ll k_2$ (133 mbar, O_2)	298	Nelson et al., 1990	(mm)
$CCl_3CH_2O + M \rightarrow CCl_3 + HCHO + M$	(2)				
$CCl_3CCl_2O + O_2 \rightarrow$ products	(1)	$k_1[O_2] \ll k_2$	298	Sato and Nakamura, 1991	(nn)
$CCl_3CCl_2O + M \rightarrow CCl_3COCl + Cl + M$	(2)				

Comments

(a) Steady-state photolysis of Cl_2 in the presence of CH_3 -air mixtures (1 atm) with FTIR absorption spectroscopic analysis: a 100% yield of HCOF was observed, consistent with $k_1[O_2] \gg k_2$,

(b) Steady-state photolysis of Cl_2 in the presence of CH_3CHF_3 -air mixtures (1 atm) with FTIR absorption spectroscopic analysis: a 100 ± 5% yield of COF_2 was observed, consistent with $k_1[O_2] \ll k_2$,

(c) Similar experiments to those of Comment (b); a 92.2 ± 1.2 % yield of COF_2 plus other identified products was observed, consistent with $k_1[O_2] \ll k_2$,

(d) Steady-state photolysis of Cl_2 in the presence of CH_3FCH_2F-air mixtures (933 mbar) with FTIR analysis: a 91± 10% yield of HCOF was observed, consistent with $k_1[O_2] \ll k_2$,

(e) Steady-state photolysis of Cl_2 in the presence of CF_3CFH_2-O_2-N_2 mixtures at total pressures of 2 atm with FTIR analysis of products CF_3COF and HCOF. The ratio k_1/k_2 was found to be pressure dependent over the range 27-732 mbar but approximately independent of pressure above 933 mbar.

(f) Similar experiments to those of Comment (e) at a total pressure of 986 mbar.

(g) Flash-photolysis time-resolved UV absorption spectroscopic study of CF_3CHFO_2 radicals from F_2-CF_3CH_2F-O_2-N_2 mixtures, k_1 obtained from a fit of CF_3O_2 formation profiles, produced from reaction (1) followed by $CF_3 + O_2 + M$. Experiments were carried out at a total pressure of 306 mbar, well below the high-pressure limit.

(h) Cl_2- initiated photooxidation of CF_3CH_2F at 1atm pressure, with dual-beam diode-array UV spectroscopic determination of CF_3COF and HCOF products.

(i) Direct time-resolved experiment using laser pulsed photolysis-laser long path absorption; CF_3CFHO produced by CF_3CFHO_2 + NO reaction and kinetics of thermal decomposition reaction determined at p = 50 mbar and ~ 300 K. The relatve rate ratio cited for k_1/k_2 was determined in a second experiment carried out over the temperature range 244-295 K and p = 100 mbar, using UV photolysis and FTIR analysis of products.

(j) Steady-state photolysis of Cl_2 in the presence of CF_3CFH_2-O_2-N_2 mixtures at total pressures of 55 - 800 mbar with FTIR analysis of products CF_3COF and HCOF. Experiments also carried out with NO present so that CF_3CFHO was produced by CF_3CFHO_2 + NO reaction, as opposed to the self reaction of CF_3CFHO_2. The ratio k_1/k_2 was found to increase with pressure over the range given but approximately independent of pressure above 1500 mbar. The ratio k_1/k_2 was significantly lower in the NO experiments. This was ascribed to the production of vibrationally hot CF_3CFHO radicals which decompose promptly to CF_3 + HCFO, in the more exothermic source reaction.

(k) Steady-state photolysis of F_2 in the presence of CF_3CFH_2-O_2-N_2 mixtures (p = 910 mbar) with FTIR absorption spectroscopic analysis.

(l) Steady-state photolysis of Cl_2 in the presence of CF_3CHF_2 -air mixtures (1 atm) with FTIR absorption spectroscopic analysis: a 109 ± 5% yield of COF_2 was observed, consistent with $k_1[O_2] \ll k_{2,}$

(m) Similar experiments to those of Comment (i) at a total pressure of 986 mbar: a ~ 100% yield of COF was observed, consistent with $k_1[O_2] \ll k_{2,}$

(n) Steady-state photolysis of Cl_2 in the presence of CH_2FCl-air mixtures (986 mbar) with FTIR absorption spectroscopic analyses: a 100% yield of HCOF was observed, consistent with $k_1[O_2] \ll k_{2,}$

(o) Steady-state photolysis of Cl_2 in the presence of CH_2FCl-air mixtures (933 mbar) with FTIR absorption spectroscopic analysis: a 111 ± 6% yield of COF_2 was observed, consistent with $k_1[O_2] \ll k_{2,}$ The cited absolute values for k_2 were derived from evaluation of data of Carr et al., (1986) and Rayez et al. (1987) reported in IUPAC Supplement IV, 1992.

(p) Similar experiments to those of Comment (l) at a total pressure of 986 mbar: a 100% yield of COF_2 was observed, consistent with $k_1[O_2] \ll k_2$. The cited absolute values for k_2 were derived from evaluation of data of Lesclaux et al. (1987) and Rayez et al. (1987) reported in IUPAC Supplement IV, 1992.

(q) Steady-state photolysis of Cl_2 in the presence of $CHFCl_2$-air mixtures (986 mbar) with FTIR absorption spectroscopic analyses: a 100% yield of COFCl was observed, consistent with $k_1[O_2] \ll k_{2,}$

(r) Steady-state photolysis of Cl_2 in the presence of $CH_2CF_2Cl_2$-air mixtures (986 mbar) with FTIR absorption spectroscopic analysis: a 100% yield of CF_2ClCHO was observed, consistent with $k_1[O_2] \gg k_{2,}$ Experiments on this reaction were also carried out by Edney and Driscoll (1992) and Tuazon and Atkinson (1993).

(s) Direct time-resolved experiment using laser pulsed photolysis-laser long path absorption; $CFCl_2CH_2O$ produced by $CFCl_2CH_2O_2$ + NO reaction.

(t) UV flash photolysis of $CFCl_2CH_3/N_2/O_2$ mixtures (13- 50 mbar); growth and decay of $CFCl_2CH_2O$ radicals in excess O_2 measured by time resolved MS.

(u) Steady-state photolysis of Cl_2 in the presence of CH_2CFCl_2-air mixtures (986 mbar) with FTIR absorption spectroscopic analysis: a 100% yield of $CFCl_2CHO$ was observed, consistent with

$k_1[O_2]$ » k_2, Experiments on this reaction were also carried out by Edney et al. (1991) and Tuazon and Atkinson (1993).

(v) Steady-state photolysis of Cl_2 in the presence of CF_3CHFCl-air mixtures (1 atm) with FTIR absorption spectroscopic analyses: a 100 ± 4% yield of CF_3COF was observed, consistent with $k_1[O_2]$ « k_2,

(w) Steady-state photolysis of Cl_2 in the presence of CF_3CHFCl-air mixtures at 986 mbar total pressure with FTIR absorption spectroscopic analyses: a 101 ± 1% yield of CF_3COF was observed, consistent with $k_1[O_2]$ » k_2,

(x) Steady-state photolysis of Cl_2 in the presence of CF_3CHCl_2-air mixtures (933 mbar) with FTIR absorption spectroscopic analyses: a ~ 100% yield of CF_3COCl was observed, consistent with $k_1[O_2]$ « k_2,

(y) Similar experiments to those of Comment (s) at a total pressure of 133 mbar. The observed formation of CF_3COCl is consistent with $k_1[O_2]$ « k_2,

(z) Similar experiments to those of Comment (s) at a total pressure of 986 mbar: a 98% yield of CF_3COCl was obseved, consistent with $k_1[O_2]$ « k_2,

(aa) Steady-state photolysis of Cl_2 in the presence of CF_3CHCl_2-air mixtures (~ 1 atm) with broad-band UV absorption analyses: a ~ 100% yield of CF_3COCl was observed, consistent with $k_1[O_2]$ « k_2,

(bb) Steady-state photolysis of Cl_2 in the presence of $CF_3CF_2CHCl_2$-air mixtures at 986 mbar with FTIR spectroscopic analyses: a 100% yield of CF_3CF_2COCl was observed, consistent with $k_1[O_2]$ « k_2,

(cc) Steady-state photolysis of Cl_2 in the presence of $CF_3ClF_2CHFCl_2$-O_2 mixtures (133 mbar) with FTIR spectroscopic analyses: observed formation of CF_2ClCF_2COF is consistent with $k_1[O_2]$ « k_2,

(dd) Steady-state photolysis of Cl_2 in the presence of CF_2ClCF_2CHFCl-O_2 mixtures (133 mbar) with FTIR spectroscopic analyses: observed formation of CF_2ClCF_2COF is consistent with $k_1[O_2]$ « k_2,

(ee) Steady-state photolysis of Cl_2 in the presence of CF_2ClCF_2CHFCl-air mixtures (986 mbar) with FTIR spectroscopic analysis: a 99% yield of CF_2ClCF_2COF was observed, consistent with $k_1[O_2]$ « k_2,

(ff) Steady-state photolysis of Cl_2 in the presence of CH_3Cl-O_2-N_2 mixtures with FTIR absorption spectroscopic analysis of HOCl, CO, HCl and $CH_2ClCOOH$ products. k_1/k_2 based on yields of CO and HOCl, the latter being corrected for secondary formation and removal. The ratio k_1/k_2 was found to be markedly pressure dependent over the range 12 to 933 mbar, and the cited value refers to 700 total pressure.

(gg) UV flash photolysis - time resolved MS. Pressure = 7 - 50 mbar; growth of HCOCl and HCl products used to determine kinetics.

(hh) Steady-state photolysis of Cl_2 in the presence of C_2H_2Cl-O_2-N_2 mixture with FTIR spectroscopic analysis of products: the observed high yields of HCL (157%) and CO_2 (53%) were explained by reaction (2)

(ii) Laser flash photolysis of Cl_2 in the presence of C_2H_5Cl-air mixtures with infrared absorption detection of HCl. The observed secondary formation of HCl was explained by reaction (2).

(jj) Steady-state photolysis of CH_3ONO or C_2H_5ONO in the presence of chloroethene -NO-air mixtures, with and without C_2H_6O as an added Cl atom scavenger. FTIR spectroscopic analysis of HCHO and HCOCl products, with close to unit yields of each. These products and their formation yields are consistent with the qualitative relative values of $k_1[O_2]$ and k_2 shown above.

(kk) Steady-state photolysis of CH_3CCl_3-O_2 mixtures in the presence of Br or NO (to scavenge Cl atoms), with GC and IR analyses of products. CH_3COCl was the major product observed, consistent with the relative values of $k_1[O_2]$ and k_2 shown above.

(ll) Steady-state photolysis of Cl_2 in the presence of CH_3CCl_3-O_2 mixtures with GC and IR analyses of CCl_3CHO and $COCl_2$, which are consistent with the relative values of $k_1[O_2]$ and k_2 shown above.

(mm) Steady-state photolysis of Cl_2 in the presence of $CHCl_2CCl_3$-O_2 mixtures (133 mbar) with FTIR spectroscopic analysis. The observed formation yields of CCl_3COCl and $COCl_2$ are consistent with the relative values of $k_1[O_2]$ and k_2 shown above.

Preferred Values

$R_1 (R_2)CHO = CF_3CHFO$
$k_1/ k_2 = 2.7 \times 10^{-20}$ cm^3 molecule^{-1} at 298 K and 1 atm pressure.
$k_1/ k_2 = 2.1 \times 10^{-25} \exp(3625/T)$ (1 bar) cm^3 molecule^{-1} over the temperature range 260-355 K.
$\Delta(E/R) = \pm500$ K.

$R_1 (R_2)CHO = CH_2ClO$
$k_1/ k_2 = 4.6 \times 10^{-18}$ cm^3 molecule^{-1} at 298 K .

Comments on Preferred Values

$R_1 (R_2)CHO = CF_3CHFO$
The recommended temperature dependence rate coefficient ratio is that evaluated by Wallington et al (1996) from their own data together with those of Wallington et al. (1992), Tuazon and Atkinson (1994), Meller et al. (1992), and Benarek et al. (1996). The data were corrected for a small pressure dependence measured by Wallington at al. (1996) at 298 K, and the expression refers to reactions of the thermalised CF_3CHFO radicals. This study also revealed that energy rich CF_3CHFO radicals were formed when the radical was produced from the CF_3CHFO_2 + NO reaction, leading to formation of HCFO by prompt decomposition at atmospheric temperatures, reducing the relative rate of O_2 reaction by a factor of 1.8 – 4.0. Several theoretical studies have investigated the decomposition of CF_3CHFO radicals and have confirmed that this interpretation is realistic. (Schneider et al., 1998; Somnitz and Zellner, 2001).

$R_1 (R_2)CHO = CH_2ClO, CH_3CHClO$
The elimination of HCl occurs from the CH_3CHClO radical (Shi et al., 1993, Maricq et al., 1993) as well as from the CH_2ClO radical (Kaiser and Wallington, 1994; Wu and Carr, 2001).

$R_1 (R_2)CHO$ = other radicals in the above table.
For the purpose of atmospheric modeling studies it is recommended that the above qualitative information on the ratios k_1/ k_2 be used to decide if one or other of the alkoxy radical reaction pathways predominates or if both pathways should be considered.

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