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

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The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 8, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, [http://iupac.pole-ether.fr](http://iupac.pole-ether.fr/).

This datasheet last evaluated: June 2014; last change in preferred values: March 2006.

**R1(R2)CHO + O2  R1COR2 + HO2 (or  products) (1)**

**R1(R2)CHO (+ M) products (2)**

# R = alkyl, halogenated alkyl, H or halogen atom

###### Rate coefficient data

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reactions | *k*1/*k*2 /cm2 molecule-1 | Temp/K | Reference | Comments |
| CH2FO + O2  HCOF + HO2 | (1) | k1[O2] » k2  (933 mbar,air) | 298 | Edney and Driscoll, 1992 | (a) |
| CH2FO + M  HCOF + H + M | (2) | k1[O2] » k2  (986 mbar,air) | 298 | Tuazon and Atkinson, 1993 | (a) |
| CH3CF2O + O2  products | (1) | k1[O2] « k2  (933 mbar,air) | 298 | Edney and Driscoll, 1992 | (b) |
| CH3CF2O + M  CH3 + COF2 + M | (2) | k1[O2] « k2  (986 mbar,air) | 298 | Tuazon and Atkinson, 1993 | (c) |
| CH2 FCHFO + O2  CH2FCOF + HO2 | (1) | k1[O2] » k2  (933 mbar,air) | 296 | Wallington et al., 1994 | (d) |
| CH2 FCHFO + M  CH2F+ HCOF+ M | (2) |  |  |  |  |
| CF3CHFO + O2  CF3COF + HO2 | (1) | 1.58 x 10-25 exp(3600/T) | 261-353 | Wallington et al., 1992 | (e) |
| CF3CHFO + M  CF3 + HCOF + M | (2) | 2.8 x 10-20 (2 atm) | 298 |  |  |
|  |  | 3.2 x 10-25 exp(3510/T) | 273-320 | Tuazon and Atkinson, 1993 | (f) |
|  |  | 4.5 x 10-20 (986 mbar) | 298 |  |  |
|  |  | k2 =3.7 x 107 exp(-2200/T)s-1 | 211-372 | Maricq and Szente, 1992 | (g) |
|  |  | k2 = 2.3 x 104 s-1 (306mbar) | 298 |  |  |
|  |  | 1.18 x 10-24 exp(2860/T) | 235-318 | Rattigan et al., 1994 | (h) |
|  |  | 1.7 x 10-20 (1 bar) | 298 |  |  |
|  |  | 1.5 x 10-19 (50 mbar) | 300 | Bednarek et al, 1996 | (i) |
|  |  | k1 = 2.7 x 10-15  | 300 |  |  |
|  |  | 8.7 x 10-25 exp(3240/T) (1 bar) | 244-295 |  |  |
|  |  | 2.1 x 10-25 exp(3625/T) (1 bar) | 238-295 | Wallington et al, 1996 | (j) |
|  |  | 1.38 x 10-24 exp(2400/T) (1 bar) | 298-357 | Hasson et al., 1998 | (k) |
| CF3CF2O + O2  products | (1) | k1[O2] « k2  (933 mbar,air) | 298 | Tuazon and Atkinson, 1993 | (e) |
| CF3CF2O + M  CF3 + CF2O + M | (2) |  |  |  |  |
| CH3CF2O + O2   products | (1) | k1[O2] « k2  (933 mbar, air) | 298  | Edney and Driscoll, 1992 | (l) |
| CH3CF2O + M  CH3 + COF2 + M | (2) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1993 | (m) |
| CHFClO + O2  COFCl + HO2 | (1) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1993 | (n) |
| CHFClO + M  HCOF + Cl + M | (2) |  |  |  |  |
| CF2ClO + O2   products | (1) | k1[O2] « k2  (933 mbar, air) | 298 | Edney and Driscoll, 1992 | (o) |
| CF2ClO + M  COF2 + Cl+ M | (2) | k2 = 7.0 x 105 | 298 | Carr et al.,(1986);Rayez et al. (1987) | FP-UVA |
|  |  | k2 = 3 x 1013exp(-5250/T) (k/s-1) |  |  |  |
| CFCl2O + O2   products | (1) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1993 | (p) |
| CFCl2O + M  COFCl + Cl+ M  | (2) | k2 = 7.0 x 105 |  | Lesclaux et al. (1987);Rayez et al. (1987) | FP-MS |
|  |  | k2 = 3 x 1013exp(-5250/T) (k/s-1) |  |  |  |
| CCl3O + M  COCl2 + Cl+ M | (2) | k2 = 8.0 x 106 |  | Lesclaux et al. (1987);Rayez et al. (1987) | FP-MS (p) |
|  |  | k2 = 4 x 1013exp(-4600/T) (k/s-1) |  |  |  |
| CF2ClCH2O + O2   CF2ClCHO+ HO2 | (1) | k1[O2] » k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1994 | (q) |
| CF2ClCH2O+M  CF2Cl + HCHO+ M | (2) |  |  |  |  |
| CFCl2CH2O + O2   CFCl2CHO+ HO2 | (1) | k1[O2] » k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1994 | (r) |
| CFCl2CH2O+M  CFCl2 + HCHO+ M | (2) |  |  |  |  |
|  |  | k1 = 2.0 x 10-15  | 298 | Mörs et al, 1996 | (s) |
|  |  | k1 = 1.3 x 10-16 | 298 | Wu and Carr, 1996 | (t) |
|  |  | k1 = 2.4 x 10-15exp[-(944 ± 55)/T] | 251-341 |  |  |
| CF3CFClO + O2   products | (1) | k1[O2] « k2  (933 mbar, air) | 298 | Edney and Driscoll, 1992 | (u) |
| CF3CFClO + M  CF3COF + Cl + M | (2) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1993 | (v) |
| CF3CCl2O + O2   products | (1) | k1[O2] « k2  (933 mbar, air) | 298 | Edney et al., 1991 | (w) |
| CF3CCl2O + M  CF3COCl + Cl + M | (2) | k1[O2] « k2  ( 135 mbar, O2) | 298 | Sato and Nakamura, 1991 | (x) |
|  |  | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1993 | (y) |
|  |  | k1[O2] « k2  (~ 1 bar, air) | 298 | Hayman et al., 1994 | (z) |
| CF3CF2CCl2O + O2   products | (1) | k1[O2] « k2  ( 135 mbar, O2) | 298 | Sato and Nakamura, 1991 | (aa) |
| CF3CF2CCl2O+MCF3CF2COCl+Cl+M | (2) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1994 | (bb) |
| CF2ClCF2CFClO + O2   products (1) | (1) | k1[O2] « k2  ( 135 mbar, O2) | 298 | Sato and Nakamura, 1991 | (cc) |
| CF2ClCF2CFClO+MCF2ClCF2COF+ Cl+M | (2) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1994 | (dd) |
| CH2ClO + O2  HCOCl + HO2 | (1) | 4.6 x 10-18 (933 mbar, O2 + N2) | 296 | Kaiser and Wallington, 1993 | (ee) |
| CH2ClO + M HCO + HCl + M | (2) | k1 = 1.3 x 10-12exp[-(934±128]/T)  | 265-306 | Wu and Carr, 2001 | (ff) |
|  |  | k2 = 7.7 x 109exp[-(4803±722]/T) (13 mbar) | 265-306 |  |  |
| CH3CHClO + O2  CH3COCl + HO2 | (1) | k1[O2] « k2  (933 mbar, air) | 295 | Shi et al., 1993 | (gg) |
| CH3CHClO + M CH3CO + HCl + M | (2) | k1[O2] « k2  (1013 mbar, air) | 298 | Maricq et al., 1993 | (hh) |
| HOCH2CHClO+O2HOCH2COCl+HCl+HO2 | (1) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1994 | (ii) |
| HOCH2CHClO+MCH2OH+HCOCl+M | (2) |  |  |  |  |
| HOCHClCH2O+O2HOCHClCHO+HO2 | (1) | k1[O2] « k2  (986 mbar, air) | 298 | Tuazon and Atkinson, 1994 | (jj) |
| HOCHClCH2O+MCHClOH+HCHO+M | (2) |  |  |  |  |
| CH3CCl2O + O2  products (1) | (1) | k1[O2] « k2  (933 mbar, O2) | 298 | Nelson et al., 1990 | (kk) |
| CH3CCl2O + M CH3COCl + Cl + M | (2) |  |  |  |  |
| CCl3CH2O + O2 CCl3CHO + HO2  | (1) | k1[O2] « k2  (133 mbar, O2) | 298 | Nelson et al., 1990 | (mm) |
| CCl3CH2O + MCCl3 + HCHO + M | (2) |  |  |  |  |
| CCl3CCl2O + O2  products | (1) | k1[O2] « k2   | 298 | Sato and Nakamura, 1991 | (nn) |
| CCl3CCl2O + M CCl3COCl + Cl + M | (2) |  |  |  |  |

##### Comments

1. Steady-state photolysis of Cl2 in the presence of CH3 -air mixtures (1 atm) with FTIR absorption spectroscopic analysis: a 100% yield of HCOF was observed, consistent with k1[O2] » k2,
2. Steady-state photolysis of Cl2 in the presence of CH3CHF3 -air mixtures (1 atm) with FTIR absorption spectroscopic analysis: a 100 ± 5% yield of COF2 was observed, consistent with k1[O2] « k2,
3. Similar experiments to those of Comment (b); a 92.2 ± 1.2 % yield of COF2 plus other identified products was observed, consistent with k1[O2] « k2,
4. Steady-state photolysis of Cl2 in the presence of CH3FCH2F-airmixtures (933 mbar) with FTIR analysis: a 91± 10% yield of HCOF was observed, consistent with k1[O2] « k2,
5. Steady-state photolysis of Cl2 in the presence of CF3CFH2-O2-N2 mixtures at total pressures of 2 atm with FTIR analysis of products CF3COF and HCOF. The ratiok1/k2 was found to be pressure dependent over the range 27-732 mbar but approximately independent of pressure above 933 mbar.
6. Similar experiments to those of Comment (e) at a total pressure of 986 mbar.
7. Flash-photolysis time-resolved UV absorption spectroscopic study of CF3CHFO2

radicals from F2-CF3CH2F-O2-N2 mixtures, k1  obtained from a fit of CF3O2 formation profiles, produced from reaction (1) followed by CF3 + O2 + M. Experiments were carried out at a total pressure of 306 mbar, well below the high-pressure limit.

1. Cl2- initiated photooxidation of CF3CH2F at 1atm pressure, with dual-beam diode-array UV spectroscopic determination of CF3COF and HCOF products.
2. Direct time-resolved experiment using laser pulsed photolysis-laser long path absorption; CF3CFHO produced by CF3CFHO2 + 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*2was 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.
3. Steady-state photolysis of Cl2 in the presence of CF3CFH2-O2-N2 mixtures at total pressures of 55 - 800 mbar with FTIR analysis of products CF3COF and HCOF. Experiments also carried out with NO present so that CF3CFHO was produced by CF3CFHO2 + NO reaction, as opposed to the self reaction of CF3CFHO2. The ratio*k1/k2* was found to increase with pressure over the range given but approximately independent of pressure above 1500 mbar. The ratio *k1/k2* was significantly lower in the NO experiments. This was ascribed to the production of vibrationally hot CF3CFHO radicals which decompose promptly to CF3 + HCFO, in the more exothermic source reaction.
4. Steady-state photolysis of F2 in the presence of CF3CFH2-O2-N2 mixtures ( p = 910 mbar) with FTIR absorption spectroscopic analysis.
5. Steady-state photolysis of Cl2 in the presence of CF3CHF2 -air mixtures (1 atm) with FTIR absorption spectroscopic analysis: a 109 ± 5% yield of COF2 was observed, consistent with k1[O2] « k2,
6. Similar experiments to those of Comment (i) at a total pressure of 986 mbar: a ~ 100% yield of COFwas observed, consistent with k1[O2] « k2,
7. Steady-state photolysis of Cl2 in the presence of CH2FCl-airmixtures (986 mbar) with FTIR absorption spectroscopic analyses: a 100% yield of HCOF was observed, consistent with k1[O2] « k2,
8. Steady-state photolysis of Cl2 in the presence of CH2FCl-airmixtures (933 mbar) with FTIR absorption spectroscopic analysis: a 111 ± 6% yield of COF2 was observed, consistent with k1[O2] « k2, The cited absolute values for k2 were derived from evaluation of data of Carr et al., (1986) and Rayez et al. (1987) reported in IUPAC Supplement IV, 1992.
9. Similar experiments to those of Comment (l) at a total pressure of 986 mbar: a 100% yield of COF2 was observed, consistent with k1[O2] « k2. The cited absolute values for k2 were derived from evaluation of data of Lesclaux et al. (1987) and Rayez et al. (1987) reported in IUPAC Supplement IV, 1992.
10. Steady-state photolysis of Cl2 in the presence of CHFCl2-airmixtures (986 mbar) with FTIR absorption spectroscopic analyses: a 100% yield of COFCl was observed, consistent with k1[O2] « k2,
11. Steady-state photolysis of Cl2 in the presence of CH2CF2Cl2-airmixtures (986 mbar) with FTIR absorption spectroscopic analysis: a 100% yield of CF2ClCHO was observed, consistent with k1[O2] » k2, Experiments on this reaction were also carried out by Edney and Driscoll (1992) and Tuazon and Atkinson (1993).
12. Direct time-resolved experiment using laser pulsed photolysis-laser long path absorption; CFCl2CH2O produced by CFCl2CH2O2 + NO reaction.
13. UV flash photolysis of CFCl2CH3/N2/O2 mixtures (13- 50 mbar); growth and decay of CFCl2CH2O radicals in excess O2 measured by time resolved MS.
14. Steady-state photolysis of Cl2 in the presence of CH2CFCl2-airmixtures (986 mbar) with FTIR absorption spectroscopic analysis: a 100% yield of CFCl2CHO was observed, consistent with k1[O2] » k2, Experiments on this reaction were also carried out by Edney et al. (1991) and Tuazon and Atkinson (1993).
15. Steady-state photolysis of Cl2 in the presence of CF3CHFCl-airmixtures (1 atm) with FTIR absorption spectroscopic analyses: a 100 ± 4% yield of CF3COF was observed, consistent with k1[O2] « k2,
16. Steady-state photolysis of Cl2 in the presence of CF3CHFCl-airmixtures at 986 mbar total pressure with FTIR absorption spectroscopic analyses: a 101 ± 1% yield of CF3COF was observed, consistent with k1[O2] » k2,
17. Steady-state photolysis of Cl2 in the presence of CF3CHCl2-airmixtures (933 mbar) with FTIR absorption spectroscopic analyses: a ~ 100% yield of CF3COCl was observed, consistent with k1[O2] « k2,
18. Similar experiments to those of Comment (s) at a total pressure of 133 mbar. The observed formation of CF3COCl is consistent with k1[O2] « k2,
19. Similar experiments to those of Comment (s) at a total pressure of 986 mbar: a 98% yield of CF3COCl was obseved, consistent with k1[O2] « k2,
20. Steady-state photolysis of Cl2 in the presence of CF3CHCl2-airmixtures (~ 1 atm) with broad-band UV absorption analyses: a ~ 100% yield of CF3COCl was observed, consistent with k1[O2] « k2,
21. Steady-state photolysis of Cl2 in the presence of CF3CF2CHCl2-airmixtures at 986 mbar with FTIR spectroscopic analyses: a 100% yield of CF3CF2COCl was observed, consistent with k1[O2] « k2,
22. Steady-state photolysis of Cl2 in the presence of CF3ClF2CHFCl2-O2 mixtures (133 mbar) with FTIR spectroscopic analyses: observed formation of CF2ClCF2COF is consistent with k1[O2] « k2,
23. Steady-state photolysis of Cl2 in the presence of CF2ClCF2CHFCl-O2 mixtures (133 mbar) with FTIR spectroscopic analyses: observed formation of CF2ClCF2COF is consistent with k1[O2] « k2,
24. Steady-state photolysis of Cl2 in the presence of CF2ClCF2CHFCl-airmixtures (986 mbar) with FTIR spectroscopic analysis: a 99% yield of CF2ClCF2COF was observed, consistent with k1[O2] « k2,
25. Steady-state photolysis of Cl2 in the presence of CH3Cl-O2-N2 mixtures with FTIR absorption spectroscopic analysis of HOCl, CO, HCl and CH2ClCOOH 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.
26. UV flash photolysis - time resolved MS. Pressure = 7 - 50 mbar; growth of HCOCl and HCl products used to determine kinetics.
27. Steady-state photolysis of Cl2 in the presence of C2H2Cl-O2-N2 mixture with FTIR spectroscopic analysis of products: the observed high yields of HCL (157%) and CO2 (53%) were explained by reaction (2)
28. Laser flash photolysis of Cl2 in the presence of C2H5Cl-air mixtures with infrared absorption detection of HCl. The observed secondary formation of HCl was explained by reaction (2).
29. Steady-state photolysis of CH3ONO or C2H5ONO in the presence of chloroethene -NO-air mixtures, with and without C2H6O 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 k1[O2] and k2 shown above.
30. Steady-state photolysis of CH3CCl3-O2 mixtures in the presence of Br or NO (to scavenge Cl atoms), with GC and IR analyses of products. CH3COCl was the major product observed, consistent with the relative values of k1[O2] and k2 shown above.
31. Steady-state photolysis of Cl2 in the presence of CH3CCl3-O2 mixtures with GC and IR analyses of CCl3CHO and COCl2, which are consistent with the relative values of k1[O2] and k2 shown above.
32. Steady-state photolysis of Cl2 in the presence of CHCl2CCl3-O2 mixtures (133 mbar) with FTIR spectroscopic analysis. The observed formation yields of CCl3COCl and COCl2 are consistent with the relative values of k1[O2] and k2 shown above.

#### Preferred Values

R1 (R2)CHO = CF3CHFO

*k*1/ *k*2 = 2.7 x 10-20 cm3 molecule-1  at 298 K and 1 atm pressure.

*k*1/ *k*2 = 2.1 x 10-25 exp(3625/T) (1 bar) cm3 molecule-1  over the temperature range 260-355 K.

∆(*E/R*) = ±500 K.

R1 (R2)CHO = CH2ClO

*k*1/ *k*2 = 4.6 x 10 -18 cm3 molecule-1  at 298 K .

*Comments on Preferred Values*

R1 (R2)CHO = CF3CHFO

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 CF3CHFO radicals. This study also revealed that energy rich CF3CHFO radicals were formed when the radical was produced from the CF3CHFO2 + NO reaction, leading to formation of HCFO by prompt decomposition at atmospheric temperatures, reducing the relative rate of O2 reaction by a factor of 1.8 – 4.0. Several theoretical studies have investigated the decomposition of CF3CHFO radicals and have confirmed that this interpretation is realistic. (Schneider et al., 1998; Somnitz and Zellner, 2001).

R1 (R2)CHO = CH2ClO, CH3CHClO

The elimination of HCl occurs from the CH3CHClO radical (Shi et al., 1993, Maricq et al., 1993) as well as from the CH2ClO radical (Kaiser and Wallington, 1994; Wu and Carr, 2001).

R1 (R2)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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