|  |  |  |  |
| --- | --- | --- | --- |
| No. | Reaction | Reaction rate | Remarks |
| 01 | Cl2+hv=2 Cl |  |  |
| 02 | HOCl+hv= Cl+OH |  |  |
| 03 | ClNO2+hv=Cl+NO2 |  |  |
| 04 | ClONO2+hv=Cl+NO3 | 0.83× |  |
| 05 | ClONO2+hv=ClO+NO2 | 0.17× |  |
| 04 | FMCl+hv=Cl+CO+HO2 |  |  |
|  | FMCl+OH=Cl + CO + H2O | 5.0E−13 |  |
| 05 | HCl+OH=Cl+H2O | 6.58E-13×(T/300)1.16×EXP(58/T) or ARRH(1.7E-12,-230.0) |  |
| 06 | Cl2+OH=HOCl+Cl | ARRH(3.6E-12,-1200.0) |  |
|  | HOCl+OH=ClO+H2O | 5.0E-13 |  |
| 07 | ClO+ClO=0.3 Cl2+1.4 Cl{+O2} | 1.63E-14 |  |
|  | ClO+NO2=ClONO2 | 7.0E-11 |  |
| 08 | ClO+NO=Cl+NO2 | ARRH(6.4E-12,290.0) |  |
| 09 | ClO+HO2=HOCl{+O2} | ARRH(2.7E-12,220.0) |  |
|  | ClO+OH=HO2+Cl | 1.8E-11 |  |
|  | ClO+OH=HCl+O2 | 1.2E-12 |  |
|  | Cl+O3=ClO{+O2} | ARRH(2.3E-11,-200.0) |  |
|  | Cl+NO2=ClNO2 | TROE(1.8E-31, 2.0, 1.0E-10, 1.0) |  |
|  | Cl+HO2=HCl{+O2} | 3.5E−11 |  |
|  | Cl+HO2=ClO+OH | ARRH(7.5E-11,-620.0) |  |
| 10 | Cl+H2O2=HCl+HO2 | ARRH(1.1E-11,-980.0) |  |
|  | Cl+NO3=NO2+ClO | 2.4E−11 |  |
|  | Cl+ClONO2=Cl2+NO3 | ARRH(6.2E-12,145.0) |  |
| 11 | Cl+CH4=HCl+CH3O2 | ARRH(6.6E-12,-1240.0) |  |
| 12 | Cl+C2H6 =HCl+0.991 ALD2+XO2+HO2 | ARRH(8.3E-11,-100.0) |  |
| 13 | Cl+PAR=HCl + XO2 + 0.11 HO2  + 0.06 ALD2 + 0.11 PAR + 0.76 RO2 | 5.0E−11 |  |
| 14 | Cl + ETH =FMCl + 2 XO2 + HO2 + HCHO | 1.07E−10 |  |
| 15 | Cl + OLE=FMCl + 0.33 ALD2 + 2 XO2 + HO2 + PAR | 2.5E−10 |  |
| 16 | Cl + OLI=0.3 HCl + 0.7 FMCl + 0.45 ALD2  + 0.3 OLE + 0.3 PAR + 1.7 XO2 + HO2 | 3.5E−10 |  |
| 17 | Cl + ISOP=0.15 HCl + XO2 + HO2 + 0.85 FMCl+ISOPRD | 4.3E−10 |  |
| 18 |  |  |  |
| 19 | Cl + HCHO=HCl + HO2 + CO | ARRH(8.2E-11,-34.0) |  |
| 20 | Cl + ALD2=HCl+C2O3 | 7.9E−11 |  |
| 21 | Cl + CH3OH=HCl+HO2+HCHO | 5.5E−11 |  |
| 22 | Cl+ANOL=HCl+HO2+ALD2 | ARRH(8.2E-11,45.0) |  |
| 23 | Cl + TOL=HCl + 0.88 XO2 + 0.88 HO2 + 0.12 NAP | 6.1E−11 |  |
| 24 | Cl + XYL=HCl + 0.84 XO2 + 0.84 HO2 + 0.16 NAP | 1.2E−10 |  |

; , where ; ; M is the number density; and T is the absolute temperature.

**Table S1.** Mechanism of chlorine chemistry in the CBMZ in WRF-Chem.

**Table xx.** Mechanism of chlorine chemistry in the CBMZ\_ReNOM in WRF-Chem.

|  |  |  |  |
| --- | --- | --- | --- |
| No. | Reaction | Reaction rate | Ref |
| 01 | Cl2 + hvCl + Cl |  | a |
| 02 | HOCl + hvCl + OH |  | a |
| 03 | ClNO2 + hvCl + NO2 |  | a |
| 04 | ClONO2 + hvCl + NO3 | 0.83× | a,b |
| 05 | ClONO2 + hvClO + NO2 | 0.17× | a,b |
| 06 | FMCl + hvCl + CO + HO2 |  | a |
| 07 | FMCl + OHCl + CO + H2O | 5.0 × 10−13 | a |
| 08 | HCl + OHCl + H2O | ARRH(1.7 × 10-12, -230.0) | a |
| 09 | Cl2 + OHHOCl + Cl | ARRH(3.6 × 10-12, -1200.0) | a |
| 10 | HOCl + OHClO + H2O | 5.0 × 10-13 | a |
| 11 | ClO + ClO0.3 Cl2 + 1.4 Cl{+O2} | 1.63 × 10-14 | a |
| 12 | ClO + NO2ClONO2 | 7.0 × 10-11 | a |
| 13 | ClO + NOCl + NO2 | ARRH(6.4 × 10-12, 290.0) | a,c |
| 14 | ClO + HO2HOCl{+O2} | ARRH(2.7 × 10-12, 220.0) | a,c |
| 15 | ClO + OHHO2 + Cl | 1.8 × 10-11 | a |
| 16 | ClO + OHHCl{+O2} | 1.2 × 10-12 | a |
| 17 | Cl + O3ClO{+O2} | ARRH(2.3 × 10-11, -200.0) | a |
| 18 | Cl + NO2ClNO2 | TROE(1.8 × 10-31, 2.0, 1.0 × 10-10, 1.0) | a |
| 19 | Cl + HO2HCl{+O2} | 3.5 × 10−11 | a |
| 20 | Cl + HO2ClO + OH | ARRH(7.5 × 10-11, -620.0) | a |
| 21 | Cl + H2O2HCl + HO2 | ARRH(1.1 × 10-11, -980.0) | a |
| 22 | Cl + NO3NO2 + ClO | 2.4 × 10−11 | a |
| 23 | Cl + ClONO2Cl2 + NO3 | ARRH(6.2 × 10-12, 145.0) | a |
| 24 | Cl + CH4HCl + CH3O2 | ARRH(6.6 × 10-12, -1240.0) | a |
| 25 | Cl + C2H6HCl + 0.991 ALD2 + XO2 + HO2 | ARRH(8.3 × 10-11, -100.0) | a |
| 26 | Cl + PARHCl + XO2 + 0.11 HO2  + 0.06 ALD2 + 0.11 PAR + 0.76 RO2 | 5.0 × 10−11 | a |
| 27 | Cl + ETHFMCl + 2 XO2 + HO2 + HCHO | 1.07 × 10−10 | a |
| 28 | Cl + OLEFMCl + 0.33 ALD2 + 2 XO2 + HO2 + PAR | 2.5 × 10−10 | a |
| 29 | Cl + OLI0.3 HCl + 0.7 FMCl + 0.45 ALD2  + 0.3 OLE + 0.3 PAR + 1.7 XO2 + HO2 | 3.5 × 10−10 | a |
| 30 | Cl + ISOP0.15 HCl + XO2 + HO2 + 0.85 FMCl+ISOPRD | 4.3 × 10−10 | a |
| 31 | Cl + HCHOHCl + HO2 + CO | ARRH(8.2 × 10-11, -34.0) | a |
| 32 | Cl + ALD2HCl + C2O3 | 7.9 × 10−11 | a |
| 33 | Cl + CH3OHHCl + HO2 + HCHO | 5.5 × 10−11 | a |
| 34 | Cl + ANOLHCl + HO2 + ALD2 | ARRH(8.2 × 10-11, 45.0) | a |
| 35 | Cl + TOLHCl + 0.88 XO2 + 0.88 HO2 + 0.12 NAP | 6.1 × 10−11 | d |
| 36 | Cl + XYLHCl + 0.84 XO2 + 0.84 HO2 + 0.16 NAP | 1.2 × 10−10 | e |

a The kinetic data are taken from the IUPAC database (<http://iupac.pole-ether.fr/index.html>); b The branching ratio is determined based on Tropospheric Ultraviolet Visible (TUV) Radiation model calculations; c Atkinson et al., (2005); d Simith et al., (2002); e Wallington et al., (1988).

; , where ; ; M is the number density; and T is the absolute temperature.



