Gas-phase reactions implemented within the CAPRAM-HM3.0.

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2			
Nr.	**Reaction**	**Rate constant**	**Reference**
G1②	Cl + C → CO[O] + HCl	$k = 6.60 \cdot 10^{-12} \exp(-1240/T)$	
G2②	Cl + CC → CCO[O] + HCl	$k = 8.30 \cdot 10^{-11} \exp(-100/T)$	
G3☒	Cl + CCC → CC(O[O])C + HCl	$k = 6.02 \cdot 10^{-11} \exp(75/T)$	
G4☒	Cl + CCC → CCCO[O] + HCl	$k = 8.26 \cdot 10^{-11} \exp(-90/T)$	
G5☒	Cl + CCCC → CCCCO[O] + HCl	$k = 9.02 \cdot 10^{-11} \exp(-120/T)$	
G6☒	Cl + CCCC → CCC(O[O])C + HCl	$k = 1.21 \cdot 10^{-10} \exp(55/T)$	
G7☒	Cl + CC(C)C → 0.564 CC(C)CO[O] + 0.436 CC(O[O])(C)C + HCl	$k = 1.43 \cdot 10^{-10}$	
G8☒	Cl + CCCCC → 0.222 CCCCCO[O] + 0.558 CCCC(O[O])C + 0.220 CCC(O[O])CC + HCl	$k = 2.80 \cdot 10^{-10}$	
G9☒	Cl + CCC(C)C → 0.408 CCC(C)CO[O] + 0.342 CC(O[O])C(C)C + 0.250 CCC(O[O])(C)C + HCl	$k = 2.20 \cdot 10^{-10}$	
G10☒	Cl + CC(C)(C)C → CC(C)(C)CO[O] + HCl	$k = 1.11 \cdot 10^{-10}$	
G11☒	Cl + CCCCCC → 0.182 CCCCCCO[O] + 0.457 CCCCC(O[O])C + 0.361 CCCC(O[O])CC + HCl	$k = 3.40 \cdot 10^{-10}$	
G12☒	Cl + CCCC(C)C → 0.321 CCCC(C)CO[O] + 0.269 CC(O[O])CC(C)C + 0.213 CCC(O[O])C(C)C + 0.197 CCCC(O[O])(C)C + HCl	$k = 2.90 \cdot 10^{-10}$	
G13☒	Cl + CCC(C)CC → 0.317 CCC(C)CCO[O] + 0.530 CC(O[O])C(C)CC + 0.153 CCC(O[O])(C)CC + HCl	$k = 2.80 \cdot 10^{-10}$	
G14☒	Cl + CCC(C)(C)C → 0.461 CC(O[O])C(C)(C)C + 0.154 CC(C)(C)CCO[O] + 0.386 CCC(C)(C)CO[O] + HCl	$k = 1.71 \cdot 10^{-10}$	
G15☒	Cl + CC(C)C(C)C →	$k = 2.30 \cdot 10^{-10}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	0.478 CC(O[O])(C)C(C)C + 0.522 CC(C)C(C)CO[O] + HCl		
G16☒	Cl + CCCCCCC → CCCCC(O[O])CC + HCl	$k = 3.90 \cdot 10^{-10}$	
G17☒	Cl + CCCCC(C)C → 0.779 CC(O[O])CCC(C)C + 0.221 CCCCC(O[O])(C)C + HCl	$k = 3.50 \cdot 10^{-10}$	
G18☒	Cl + CCCC(C)CC → 0.793 CC(O[O])CC(C)CC + 0.207 CCCC(O[O])(C)CC + HCl	$k = 3.11 \cdot 10^{-10}$	
G19☒	Cl + CCCCCCCC → CCCCCC(O[O])CC + HCl	$k = 4.60 \cdot 10^{-10}$	
G20☒	Cl + CCCCCCCCC → CCCCCCC(O[O])CC + HCl	$k = 4.80 \cdot 10^{-10}$	
G21☒	Cl + CCCCCCCCCC → CCCCCCCC(O[O])CC + HCl	$k = 5.55 \cdot 10^{-10}$	
G22☒	Cl + CCCCCCCCCCC → CCCCCCCCC(O[O])CC + HCl	$k = 6.17 \cdot 10^{-10}$	
G23☒	Cl + CCCCCCCCCCCC → CCCCCCCCCC(O[O])CC + HCl	$k = 6.74 \cdot 10^{-10}$	
G24☒	Cl + C1CCCCC1 → C1CCC(O[O])CC1 + HCl	$k = 3.50 \cdot 10^{-10}$	
G25②	CCl + OH → ClCO[O] + H_2O	$k = 7.33 \cdot 10^{-18} * T^2 \exp(-809/T)$	
G26②	ClCCl + OH → [O]OC(Cl)Cl + H_2O	$k = 6.14 \cdot 10^{-18} * T^2 \exp(-389/T)$	
G27②	ClC(Cl)Cl + OH → [O]OC(Cl)(Cl)Cl + H_2O	$k = 1.80 \cdot 10^{-18} * T^2 \exp(-129/T)$	
G28②	CC(Cl)(Cl)Cl + OH → ClC(Cl)(Cl)CO[O] + H_2O	$k = 2.25 \cdot 10^{-18} * T^2 \exp(-910/T)$	
G29②	ClC(Cl)=C(Cl)Cl + OH → OC(Cl)(Cl)C(Cl)(Cl)O[O]	$k = 3.50 \cdot 10^{-12} \exp(-920/T)$	
G30②	ClC(Cl)=CCl + OH → 0.50 OC(Cl)C(Cl)(Cl)O[O] + 0.50 OC(Cl)(Cl)C(Cl)O[O]	$k = 3.00 \cdot 10^{-13} \exp(565/T)$	
G31☒	Cl/C=C\Cl + OH → OC(Cl)C(Cl)O[O]	$k = 1.94 \cdot 10^{-12} \exp(90/T)$	
G32☒	Cl/C=C/Cl + OH → OC(Cl)C(Cl)O[O]	$k = 1.01 \cdot 10^{-12} \exp(250/T)$	
G33☒	ClCCCl + OH → ClCC(Cl)O[O] + H_2O	$k = 8.69 \cdot 10^{-12} \exp(-1070/T)$	
G34☒	ClC(Cl)=C + OH → 0.50 OCC(Cl)(Cl)O[O] + 0.50 OC(Cl)(Cl)CO[O]	$k = 2.00 \cdot 10^{-12} \exp(506/T)$	
G35☒	CC(Cl)CCl + OH →	$k = 4.42 \cdot 10^{-13}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	0.11 ClCC(Cl)CO[O] + 0.6 CC(Cl)(O[O])CCl + 0.29 CC(Cl)C(Cl)O[O] + H_2O		
G36☒	CC(Cl)Cl + OH → 0.85 CC(Cl)(Cl)O[O] + 0.15 ClC(Cl)CO[O] + H_2O	$k = 2.00 \cdot 10^{-12} \exp(-596/T)$	
G37☒	CCCl + OH → 0.87 ClCCO[O] + 0.13 CC(Cl)O[O] + H_2O	$k = 7.78 \cdot 10^{-18} * T^2 \exp(-152/T)$	
G38☒	ClC(Cl)C(Cl)Cl + OH → ClC(Cl)C(Cl)(Cl)O[O] + H_2O	$k = 5.13 \cdot 10^{-13}$	
G39☒	ClC(Cl)CCl + OH → 0.5 ClCC(Cl)(Cl)O[O] + 0.5 ClC(Cl)C(Cl)O[O] + H_2O	$k = 4.44 \cdot 10^{-18} * T^2 \exp(-208/T)$	
G40☒	ClC=C + NO_3 → 0.35 ClC(ON(=O)=O)CO[O] + 0.65 [O]OC(Cl)CON(=O)=O	$k = 2.30 \cdot 10^{-16}$	
G41☒	ClC=C + O_3 → 0.76 O=CCl + 0.76 [O-][O+]=C*b + 0.24 C=O + 0.24 [O-][O+]=CCl*a	$k = 2.45 \cdot 10^{-19}$	
G42☒	ClC=C + OH → 0.50 OC(Cl)CO[O] + 0.50 OCC(Cl)O[O]	$k = 8.49 \cdot 10^{-12}$	
G43②	ClCO[O] + HO_2 → 0.3 ClCOO + 0.7 O=CCl	$k = 3.20 \cdot 10^{-13} \exp(820/T)$	
G44②	ClCO[O] + NO → ClC[O] + NO_2	$k = 4.05 \cdot 10^{-12} \exp(360/T)$	implemented from MCM
G45☒	ClCO[O] + NO_3 → ClC[O] + NO_2	$k = 2.30 \cdot 10^{-12}$	
G46②	ClCO[O] → 0.6 ClC[O] + 0.2 OCCl + 0.2 O=CCl	$k = 2.80 \cdot 10^{-13} \exp(618/T) * RO_2$	implemented from MCM
G47②	[O]OC(Cl)Cl + HO_2 → OOC(Cl)Cl	$k = 5.60 \cdot 10^{-13} \exp(700/T)$	
G48②	[O]OC(Cl)Cl + NO → [O]C(Cl)Cl + NO_2	$k = 4.05 \cdot 10^{-12} \exp(360/T)$	implemented from MCM
G49☒	[O]OC(Cl)Cl + NO_3 → [O]C(Cl)Cl + NO_2	$k = 2.30 \cdot 10^{-12}$	
G50②	[O]OC(Cl)Cl → 0.6 [O]C(Cl)Cl + 0.2 OC(Cl)Cl + 0.2 O=C(Cl)Cl	$k = 2.00 \cdot 10^{-12} * RO_2$	implemented from MCM
G51②	[O]OC(Cl)(Cl)Cl + HO_2 → OOC(Cl)(Cl)Cl	$k = 4.70 \cdot 10^{-13} \exp(710/T)$	implemented from MCM
G52②	[O]OC(Cl)(Cl)Cl + NO → [O]C(Cl)(Cl)Cl + NO_2	$k = 4.86 \cdot 10^{-12} \exp(360/T)$	implemented from MCM
G53☒	[O]OC(Cl)(Cl)Cl + NO_3 → [O]C(Cl)(Cl)Cl + NO_2	$k = 2.30 \cdot 10^{-12}$	
G54②	[O]OC(Cl)(Cl)Cl → 0.7 [O]C(Cl)(Cl)Cl + 0.3 OC(Cl)(Cl)Cl	$k = 3.69 \cdot 10^{-13} \exp(553/T) * RO_2$	implemented from MCM
G55☒	ClC(Cl)(Cl)CO[O] + HO_2 → ClC(Cl)(Cl)COO	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G56②	ClC(Cl)(Cl)CO[O] + NO → ClC(Cl)(Cl)C[O] + NO_2	$k = 4.05 \cdot 10^{-12} \exp(360/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G57☒	ClC(Cl)(Cl)CO[O] + NO_3 → ClC(Cl)(Cl)C[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G58②	ClC(Cl)(Cl)CO[O] → 0.6 ClC(Cl)(Cl)C[O] + 0.2 OCC(Cl)(Cl)Cl + 0.2 ClC(Cl)(Cl)C=O	k = $2.00 \cdot 10^{-12}$*RO_2	implemented from MCM
G59☒	OC(Cl)(Cl)C(Cl)(Cl)O[O] + HO_2 → OC(Cl)(Cl)C(Cl)(Cl)OO	k = $3.30 \cdot 10^{-13}$exp(820/T)	
G60②	OC(Cl)(Cl)C(Cl)(Cl)O[O] + NO → OC(Cl)(Cl)C(Cl)(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12}$exp(360/T)	implemented from MCM
G61☒	OC(Cl)(Cl)C(Cl)(Cl)O[O] + NO_3 → OC(Cl)(Cl)C(Cl)(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G62②	OC(Cl)(Cl)C(Cl)(Cl)O[O] → 0.3 OC(Cl)(Cl)C(O)(Cl)Cl + 0.7 OC(Cl)(Cl)C(Cl)(Cl)[O]	k = $9.20 \cdot 10^{-14}$*RO_2	implemented from MCM
G63☒	OC(Cl)C(Cl)(Cl)O[O] + HO_2 → OC(Cl)C(Cl)(Cl)OO	k = $3.30 \cdot 10^{-13}$exp(820/T)	
G64②	OC(Cl)C(Cl)(Cl)O[O] + NO → OC(Cl)C(Cl)(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12}$exp(360/T)	implemented from MCM
G65☒	OC(Cl)C(Cl)(Cl)O[O] + NO_3 → OC(Cl)C(Cl)(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G66②	OC(Cl)C(Cl)(Cl)O[O] → 0.3 OC(Cl)(Cl)C(O)Cl + 0.7 OC(Cl)C(Cl)(Cl)[O]	k = $9.20 \cdot 10^{-14}$*RO_2	implemented from MCM
G67☒	OC(Cl)(Cl)C(Cl)O[O] + HO_2 → OC(Cl)(Cl)C(Cl)OO	k = $3.30 \cdot 10^{-13}$exp(820/T)	
G68②	OC(Cl)(Cl)C(Cl)O[O] + NO → OC(Cl)(Cl)C(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12}$exp(360/T)	implemented from MCM
G69☒	OC(Cl)(Cl)C(Cl)O[O] + NO_3 → OC(Cl)(Cl)C(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G70②	OC(Cl)(Cl)C(Cl)O[O] → 0.2 OC(Cl)(Cl)C(O)Cl + 0.6 OC(Cl)(Cl)C(Cl)[O] + 0.2 OC(Cl)(Cl)C(=O)Cl	k = $8.80 \cdot 10^{-13}$*RO_2	implemented from MCM
G71☒	OC(Cl)C(Cl)O[O] + HO_2 → OC(Cl)C(Cl)OO	k = $3.30 \cdot 10^{-13}$exp(820/T)	
G72☒	OC(Cl)C(Cl)O[O] + NO → OC(Cl)C(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12}$exp(360/T)	
G73☒	OC(Cl)C(Cl)O[O] + NO_3 → OC(Cl)C(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G74☒	OC(Cl)C(Cl)O[O] → 0.2 OC(Cl)C(O)Cl + 0.6 OC(Cl)C(Cl)[O] + 0.2 OC(Cl)C(=O)Cl	k = $8.80 \cdot 10^{-13}$*RO_2	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G75☒	ClCC(Cl)O[O] + HO_2 → ClCC(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G76☒	ClCC(Cl)O[O] + NO → ClCC(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G77☒	ClCC(Cl)O[O] + NO_3 → ClCC(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G78☒	ClCC(Cl)O[O] → 0.2 ClCC=O + 0.6 ClCC(Cl)[O] + 0.2 ClCC(O)Cl	k = $8.80 \cdot 10^{-13}$*RO_2	
G79☒	OCC(Cl)(Cl)O[O] + HO_2 → OOCl.OCCCl	k = $2.91 \cdot 10^{-13} \exp(1300/T)$	
G80☒	OCC(Cl)(Cl)O[O] + NO → OCC(Cl)(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G81☒	OCC(Cl)(Cl)O[O] + NO_3 → OCC(Cl)(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G82☒	OCC(Cl)(Cl)O[O] → 0.7 OCC(Cl)(Cl)[O] + 0.3 OCC(O)(Cl)Cl	k = $8.80 \cdot 10^{-13}$*RO_2	
G83☒	OC(Cl)(Cl)CO[O] + HO_2 → OC(Cl)(Cl)COO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G84☒	OC(Cl)(Cl)CO[O] + NO → OC(Cl)(Cl)C[O] + NO_2	k = $3.24 \cdot 10^{-12} \exp(360/T)$	
G85☒	OC(Cl)(Cl)CO[O] + NO_3 → OC(Cl)(Cl)C[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G86☒	OC(Cl)(Cl)CO[O] → 0.6 OC(Cl)(Cl)C[O] + 0.2 OCC(O)(Cl)Cl + 0.2 OC(Cl)(Cl)C=O	k = $2.00 \cdot 10^{-12}$*RO_2	
G87☒	ClCC(Cl)CO[O] + HO_2 → ClCC(Cl)COO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G88☒	ClCC(Cl)CO[O] + NO → ClCC(Cl)C[O] + NO_2	k = $2.70 \cdot 10^{-12} \exp(360/T)$	
G89☒	ClCC(Cl)CO[O] + NO_3 → ClCC(Cl)C[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G90☒	ClCC(Cl)CO[O] → 0.6 ClCC(Cl)C[O] + 0.2 OCC(Cl)CCl + 0.2 ClCC(Cl)C=O	k = $2.00 \cdot 10^{-12}$*RO_2	
G91☒	CC(Cl)(O[O])CCl + HO_2 → CC(Cl)(OO)CCl	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G92☒	CC(Cl)(O[O])CCl + NO → CC(Cl)([O])CCl + NO_2	k = $2.70 \cdot 10^{-12} \exp(360/T)$	
G93☒	CC(Cl)(O[O])CCl + NO_3 → CC(Cl)([O])CCl + NO_2	k = $2.30 \cdot 10^{-12}$	
G94☒	CC(Cl)(O[O])CCl → 0.7 CC(Cl)([O])CCl + 0.3 CC(O)(Cl)CCl	k = $9.20 \cdot 10^{-13}$*RO_2	
G95☒	CC(Cl)C(Cl)O[O] + HO_2 → CC(Cl)C(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G96☒	CC(Cl)C(Cl)O[O] + NO → CC(Cl)C(Cl)[O] + NO_2	k = $2.70 \cdot 10^{-12} \exp(360/T)$	
G97☒	CC(Cl)C(Cl)O[O] + NO_3 → CC(Cl)C(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G98☒	CC(Cl)C(Cl)O[O] →	k = $8.80 \cdot 10^{-13}$*RO_2	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	0.2 CC(Cl)C(=O)Cl + 0.6 CC(Cl)C(Cl)[O] + 0.2 CC(Cl)C(O)Cl		
G99☒	CC(Cl)(Cl)O[O] + HO_2 → CC(Cl)(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G100☒	CC(Cl)(Cl)O[O] + NO → CC(Cl)(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G101☒	CC(Cl)(Cl)O[O] + NO_3 → CC(Cl)(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G102☒	CC(Cl)(Cl)O[O] → 0.7 CC(Cl)(Cl)[O] + 0.3 CC(O)(Cl)Cl	k = $9.20 \cdot 10^{-14} * RO_2$	
G103☒	ClC(Cl)CO[O] + HO_2 → ClC(Cl)COO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G104☒	ClC(Cl)CO[O] + NO → ClC(Cl)C[O] + NO_2	k = $3.24 \cdot 10^{-12} \exp(360/T)$	
G105☒	ClC(Cl)CO[O] + NO_3 → ClC(Cl)C[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G106☒	ClC(Cl)CO[O] → 0.6 ClC(Cl)C[O] + 0.2 ClC(Cl)C=O + 0.2 OCC(Cl)Cl	k = $2.00 \cdot 10^{-12} * RO_2$	
G107☒	ClCCO[O] + HO_2 → ClCCOO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G108②	ClCCO[O] + NO → ClCC[O] + NO_2	k = $3.24 \cdot 10^{-12} \exp(360/T)$	implemented from MCM
G109☒	ClCCO[O] + NO_3 → ClCC[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G110②	ClCCO[O] → 0.6 ClCC[O] + 0.2 OCCCl + 0.2 ClCC=O	k = $1.32 \cdot 10^{-13} \exp(833/T)$	implemented from MCM
G111☒	CC(Cl)O[O] + HO_2 → CC(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G112☒	CC(Cl)O[O] + NO → CC(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G113☒	CC(Cl)O[O] + NO_3 → CC(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G114☒	CC(Cl)O[O] → 0.6 CC(Cl)[O] + 0.2 CC(O)Cl + 0.2 CC(=O)Cl	k = $2.65 \cdot 10^{-12} * RO_2$	
G115☒	ClC(Cl)C(Cl)(Cl)O[O] + HO_2 → ClC(Cl)C(Cl)(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G116☒	ClC(Cl)C(Cl)(Cl)O[O] + NO → ClC(Cl)C(Cl)(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G117☒	ClC(Cl)C(Cl)(Cl)O[O] + NO_3 → ClC(Cl)C(Cl)(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G118☒	ClC(Cl)C(Cl)(Cl)O[O] → 0.7 ClC(Cl)C(Cl)(Cl)[O] + 0.3 ClC(Cl)C(O)(Cl)Cl	k = $9.20 \cdot 10^{-14} * RO_2$	
G119☒	ClCC(Cl)(Cl)O[O] + HO_2 → ClCC(Cl)(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G120☒	ClCC(Cl)(Cl)O[O] + NO → ClCC(Cl)(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G121☒	ClCC(Cl)(Cl)O[O] + NO_3 → ClCC(Cl)(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G122☒	ClCC(Cl)(Cl)O[O] →	k = $9.20 \cdot 10^{-14} * RO_2$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	0.6 ClCC(Cl)(Cl)[O] + 0.2 ClCC(O)(Cl)Cl + 0.2 ClCC(=O)Cl		
G123☒	ClC(Cl)C(Cl)O[O] + HO_2 → ClC(Cl)C(Cl)OO	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G124☒	ClC(Cl)C(Cl)O[O] + NO → ClC(Cl)C(Cl)[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G125☒	ClC(Cl)C(Cl)O[O] + NO_3 → ClC(Cl)C(Cl)[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G126☒	ClC(Cl)C(Cl)O[O] → 0.2 ClC(Cl)C=O + 0.6 ClC(Cl)C(Cl)[O] + 0.2 ClC(Cl)C(O)Cl	k = $2.00 \cdot 10^{-12} * RO_2$	
G127☒	ClC(ON(=O)=O)CO[O] + HO_2 → ClC(ON(=O)=O)COO + OH	k = $1.13 \cdot 10^{-13} \exp(1300/T)$	
G128☒	ClC(ON(=O)=O)CO[O] + NO → ClC(ON(=O)=O)C[O] + NO_2	k = $4.32 \cdot 10^{-12} \exp(360/T)$	
G129☒	ClC(ON(=O)=O)CO[O] + NO_3 → ClC(ON(=O)=O)C[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G130☒	ClC(ON(=O)=O)CO[O] → 0.2 ClC(ON(=O)=O)C=O + 0.6 ClC(ON(=O)=O)C[O] + 0.2 OCC(Cl)ON(=O)=O	k = $2.00 \cdot 10^{-12} * RO_2$	
G131☒	[O]OC(Cl)CON(=O)=O + HO_2 → OOC(Cl)CON(=O)=O + OH	k = $3.30 \cdot 10^{-13} \exp(820/T)$	
G132☒	[O]OC(Cl)CON(=O)=O + NO → [O]C(Cl)CON(=O)=O + NO_2	k = $5.94 \cdot 10^{-12} \exp(360/T)$	
G133☒	[O]OC(Cl)CON(=O)=O + NO_3 → [O]C(Cl)CON(=O)=O + NO_2	k = $2.30 \cdot 10^{-12}$	
G134☒	[O]OC(Cl)CON(=O)=O → 0.6 [O]C(Cl)CON(=O)=O + 0.2 OC(Cl)CON(=O)=O + 0.2 O=C(Cl)CON(=O)=O	k = $2.00 \cdot 10^{-12} * RO_2$	
G135☒	O=CCl + NO_3 → CO + Cl + HNO_3	k = $1.40 \cdot 10^{-12} \exp(-1860/T)$	
G136②	O=CCl + OH → CO + Cl + H_2O	k = $6.12 \cdot 10^{-12}$	implemented from MCM
G137②	O=CCl → HO_2 + CO + Cl	J = $4.642 \cdot 10^{-05} * \cos(\chi)^{0.762} \exp(-0.353/\cos(\chi))$	implemented from MCM
G138☒	[O-][O+]=CCl*a → 0.25 [O-][O+]=CCl + 0.395 HCl + 0.395 HO_2 + 0.395 Cl + 0.355 OH + 0.355 CO + 0.355 Cl	k = $1.00 \cdot 10^{+06}$	
G139☒	OC(Cl)CO[O] + HO_2 → OC(Cl)COO	k = $1.13 \cdot 10^{-13} \exp(1300/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G140☒	$OC(Cl)CO[O] + NO \rightarrow OC(Cl)C[O] + NO_2$	$k = 4.32 \cdot 10^{-12} \exp(360/T)$	
G141☒	$OC(Cl)CO[O] + NO_3 \rightarrow OC(Cl)C[O] + NO_2$	$k = 2.30 \cdot 10^{-12}$	
G142☒	$OC(Cl)CO[O] \rightarrow$ 0.2 $OC(Cl)C{=}O$ + 0.2 $OCC(O)Cl$ + 0.6 $OC(Cl)C[O]$	$k = 2.00 \cdot 10^{-12} * RO_2$	
G143☒	$OCC(Cl)O[O] + HO_2 \rightarrow OCC(Cl)OO$	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G144☒	$OCC(Cl)O[O] + NO \rightarrow OCC(Cl)[O] + NO_2$	$k = 5.94 \cdot 10^{-12} \exp(360/T)$	
G145☒	$OCC(Cl)O[O] + NO_3 \rightarrow OCC(Cl)[O] + NO_2$	$k = 2.30 \cdot 10^{-12}$	
G146☒	$OCC(Cl)O[O] \rightarrow$ 0.6 $OCC(Cl)[O]$ + 0.2 $OCC(O)Cl$ + 0.2 $OCC(=O)Cl$	$k = 8.80 \cdot 10^{-13} * RO_2$	
G147☒	$ClCOO + OH \rightarrow ClCO[O] + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G148②	$ClCOO + OH \rightarrow O{=}CCl + OH + H_2O$	$k = 4.14 \cdot 10^{-12}$	implemented from MCM
G149②	$ClCOO \rightarrow ClC[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	implemented from MCM
G150②	$ClC[O] + O_2 \rightarrow O{=}CCl + HO_2$	$k = 2.50 \cdot 10^{-14} \exp(-300/T)$	implemented from MCM
G151②	$OCCl + OH \rightarrow O{=}CCl + HO_2 + H_2O$	$k = 1.08 \cdot 10^{-12}$	
G152☒	$OOC(Cl)Cl + OH \rightarrow [O]OC(Cl)Cl + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G153☒	$OOC(Cl)Cl + OH \rightarrow O{=}C(Cl)Cl + OH + H_2O$	$k = 3.44 \cdot 10^{-12}$	
G154☒	$OOC(Cl)Cl \rightarrow [O]C(Cl)Cl + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G155☒	$[O]C(Cl)Cl + O_2 \rightarrow O{=}CCl + Cl$	$k = 1.00 \cdot 10^{+06}$	
G156②	$OC(Cl)Cl + OH \rightarrow O{=}C(Cl)Cl + HO_2 + H_2O$	$k = 9.34 \cdot 10^{-13}$	
G157☒	$O{=}C(Cl)Cl \rightarrow CO + Cl + Cl$	$J = 2.792 \cdot 10^{-05} * \cos(\chi)^{0.805} \exp(-0.338/\cos(\chi))$	
G158☒	$OOC(Cl)(Cl)Cl + OH \rightarrow [O]OC(Cl)(Cl)Cl + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G159☒	$OOC(Cl)(Cl)Cl \rightarrow [O]C(Cl)(Cl)Cl + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G160②	$[O]C(Cl)(Cl)Cl + O_2 \rightarrow O{=}C(Cl)Cl + Cl$	$k = 1.00 \cdot 10^{+06}$	implemented from MCM
G161②	$OC(Cl)(Cl)Cl + OH \rightarrow [O]C(Cl)(Cl)Cl + H_2O$	$k = 3.60 \cdot 10^{-14}$	
G162☒	$ClC(Cl)(Cl)COO + OH \rightarrow ClC(Cl)(Cl)CO[O]$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G163☒	$ClC(Cl)(Cl)COO + OH \rightarrow ClC(Cl)(Cl)C{=}O + OH$	$k = 9.80 \cdot 10^{-13}$	
G164☒	$ClC(Cl)(Cl)COO \rightarrow ClC(Cl)(Cl)C[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G165②	$ClC(Cl)(Cl)C[O] + O_2 \rightarrow ClC(Cl)(Cl)C{=}O + HO_2$	$k = 2.50 \cdot 10^{-14} \exp(-300/T)$	implemented from MCM
G166②	$OCC(Cl)(Cl)Cl + OH \rightarrow$ $ClC(Cl)(Cl)C{=}O + HO_2 + H_2O$	$k = 2.56 \cdot 10^{-12}$	
G167☒	$ClC(Cl)(Cl)C{=}O + NO_3 \rightarrow$ $ClC(Cl)(Cl)C(=O)O[O] + HNO_3$	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	
G168②	$ClC(Cl)(Cl)C{=}O + OH \rightarrow$	$k = 1.45 \cdot 10^{-12}$	implemented from MCM

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	ClC(Cl)(Cl)C(=O)O[O] + H_2O		
G169②	ClC(Cl)(Cl)C=O → [O]OC(Cl)(Cl)Cl + HO_2 + CO	J = $4.642 \cdot 10^{-05}$*cos(χ)$^{0.762}$exp(-0.353/cos(χ))	implemented from MCM
G170☒	OC(Cl)(Cl)C(Cl)(Cl)OO + OH → OC(Cl)(Cl)C(Cl)(Cl)O[O] + H_2O	k = $3.63 \cdot 10^{-12}$	
G171☒	OC(Cl)(Cl)C(Cl)(Cl)OO → OC(Cl)(Cl)C(Cl)(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G172☒	OC(Cl)(Cl)C(Cl)(Cl)[O] → O=C(Cl)Cl + O=C(Cl)Cl + HO_2	k = $1.00 \cdot 10^{+06}$	
G173②	OC(Cl)(Cl)C(O)(Cl)Cl + OH → OC(Cl)(Cl)C(Cl)(Cl)[O] + H_2O	k = $7.18 \cdot 10^{-14}$	
G174☒	OC(Cl)C(Cl)(Cl)OO + OH → OC(Cl)C(Cl)(Cl)O[O] + H_2O	k = $3.84 \cdot 10^{-12}$	
G175☒	OC(Cl)C(Cl)(Cl)OO → OC(Cl)C(Cl)(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G176☒	OC(Cl)C(Cl)(Cl)[O] → O=C(Cl)Cl + O=CCl + HO_2	k = $1.00 \cdot 10^{+06}$	
G177②	OC(Cl)(Cl)C(O)Cl + OH → OC(Cl)(Cl)C(=O)Cl + HO_2 + H_2O	k = $2.85 \cdot 10^{-13}$	
G178☒	OC(Cl)(Cl)C(Cl)OO + OH → OC(Cl)(Cl)C(Cl)O[O] + H_2O	k = $4.44 \cdot 10^{-12}$	
G179☒	OC(Cl)(Cl)C(Cl)OO → OC(Cl)(Cl)C(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G180☒	OC(Cl)(Cl)C(Cl)[O] → O=C(Cl)Cl + O=CCl + HO_2	k = $1.00 \cdot 10^{+06}$	
G181②	OC(Cl)(Cl)C(=O)Cl + OH → O=C(Cl)Cl + CO + Cl + H_2O	k = $3.59 \cdot 10^{-14}$	
G182②	OC(Cl)(Cl)C(=O)Cl → O=C(Cl)Cl + CO + Cl + HO2	J = $2.792 \cdot 10^{-05}$*cos(χ)$^{0.805}$exp(-0.338/cos(χ))	implemented from MCM
G183☒	OC(Cl)C(Cl)OO + OH → OC(Cl)C(Cl)O[O] + H_2O	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G184☒	OC(Cl)C(Cl)OO + OH → OC(Cl)C(=O)Cl + OH + H_2O	k = $6.54 \cdot 10^{-12}$	
G185☒	OC(Cl)C(Cl)OO → OC(Cl)C(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G186☒	OC(Cl)C(Cl)[O] → O=CCl + O=CCl + HO_2	k = $1.00 \cdot 10^{+06}$	
G187☒	OC(Cl)C(O)Cl + OH → OC(Cl)C(=O)Cl + HO_2 + H_2O	k = $2.77 \cdot 10^{-12}$	
G188☒	OC(Cl)C(=O)Cl + OH → O=C(Cl)C(=O)Cl + HO_2 + H_2O	k = $1.84 \cdot 10^{-12}$	
G189☒	OC(Cl)C(=O)Cl → O=CCl + O=CCl + HO_2	J = $2.792 \cdot 10^{-05}$*cos(χ)$^{0.805}$exp(-0.338/cos(χ))	
G190☒	ClCC(Cl)OO + OH → ClCC(Cl)O[O] + H_2O	k = $1.16 \cdot 10^{-11}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G191☒	$ClCC(Cl)OO \rightarrow ClCC(Cl)[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G192☒	$ClCC(Cl)[O] \rightarrow ClCC{=}O + Cl$	$k = 1.00 \cdot 10^{+06}$	
G193☒	$ClCC{=}O + NO_3 \rightarrow ClCC(=O)O[O] + HNO_3$	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	
G194②	$ClCC{=}O + OH \rightarrow ClCC(=O)O[O] + H_2O$	$k = 2.09 \cdot 10^{-11}$	implemented from MCM
G195②	$ClCC{=}O \rightarrow ClCO[O] + HO_2 + CO$	$J = 4.642 \cdot 10^{-05} * \cos(\chi)^{0.762} \exp(-0.353/\cos(\chi))$	implemented from MCM
G196☒	$ClCC(O)Cl + OH \rightarrow ClCC(Cl)[O] + H_2O$	$k = 3.75 \cdot 10^{-12}$	
G197☒	$OOClOCCCl + OH \rightarrow OCC(Cl)(Cl)O[O] + H_2O$	$k = 4.91 \cdot 10^{-12}$	
G198☒	$OOClOCCCl \rightarrow OCC(Cl)(Cl)[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G199☒	$OCC(Cl)(Cl)[O] + O_2 \rightarrow O{=}C(Cl)Cl + C{=}O + HO_2$	$k = 1.00 \cdot 10^{+06}$	
G200☒	$OCC(O)(Cl)Cl + OH \rightarrow OCC(Cl)(Cl)[O] + H_2O$	$k = 1.46 \cdot 10^{-12}$	
G201☒	$OCC(O)(Cl)Cl + OH \rightarrow OC(Cl)(Cl)C{=}O + HO_2 + H_2O$	$k = 1.10 \cdot 10^{-12}$	
G202☒	$OC(Cl)(Cl)COO + OH \rightarrow OC(Cl)(Cl)CO[O] + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G203☒	$OC(Cl)(Cl)COO + OH \rightarrow OC(Cl)(Cl)C{=}O + OH + H_2O$	$k = 6.55 \cdot 10^{-12}$	
G204☒	$OC(Cl)(Cl)COO \rightarrow OC(Cl)(Cl)C[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G205☒	$OC(Cl)(Cl)C[O] + O_2 \rightarrow C{=}O + O{=}C(Cl)Cl + HO_2$	$k = 1.00 \cdot 10^{+06}$	
G206☒	$OC(Cl)(Cl)C{=}O + NO_3 \rightarrow OC(Cl)(Cl)C(=O)O[O] + HNO_3$	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	
G207☒	$OC(Cl)(Cl)C{=}O + OH \rightarrow OC(Cl)(Cl)C(=O)O[O]$	$k = 6.18 \cdot 10^{-12}$	
G208☒	$OC(Cl)(Cl)C{=}O \rightarrow O{=}C(Cl)Cl + 2\ HO_2 + CO$	$J = 7.914 \cdot 10^{-05} * \cos(\chi)^{0.764} \exp(-0.364/\cos(\chi))$	
G209☒	$ClCC(Cl)COO + OH \rightarrow ClCC(Cl)CO[O] + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G210☒	$ClCC(Cl)COO + OH \rightarrow ClCC(Cl)C{=}O + OH + H_2O$	$k = 6.87 \cdot 10^{-12}$	
G211☒	$ClCC(Cl)COO \rightarrow ClCC(Cl)C[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G212☒	$ClCC(Cl)C[O] \rightarrow ClCC(Cl)C{=}O + HO_2$	$k = 2.50 \cdot 10^{-14} \exp(-300/T)$	
G213☒	$OCC(Cl)CCl + OH \rightarrow ClCC(Cl)C{=}O + HO_2 + H_2O$	$k = 1.10 \cdot 10^{-12}$	
G214☒	$ClCC(Cl)C{=}O + NO_3 \rightarrow ClCC(Cl)C(=O)O[O] + HNO_3$	$k = 3.36 \cdot 10^{-12} \exp(-1860/T)$	
G215☒	$ClCC(Cl)C{=}O + OH \rightarrow ClCC(Cl)C(=O)O[O] + H_2O$	$k = 7.63 \cdot 10^{-12}$	
G216☒	$ClCC(Cl)C{=}O \rightarrow ClCC(Cl)O[O] + HO_2 + CO$	$J = 7.914 \cdot 10^{-05} * \cos(\chi)^{0.764} \exp(-0.364/\cos(\chi))$	
G217☒	$CC(Cl)(OO)CCl + OH \rightarrow CC(Cl)(O[O])CCl + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G218☒	$CC(Cl)(OO)CCl \rightarrow CC(Cl)([O])CCl + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G219☒	$CC(Cl)([O])CCl \rightarrow CC(=O)CCl + Cl$	$k = 1.00 \cdot 10^{+06}$	
G220☒	$CC(O)(Cl)CCl + OH \rightarrow CC(Cl)([O])CCl + H_2O$	$k = 7.44 \cdot 10^{-13}$	
G221☒	$CC(Cl)C(Cl)OO + OH \rightarrow CC(Cl)C(=O)Cl + OH + H_2O$	$k = 6.08 \cdot 10^{-12}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G222☒	CC(Cl)C(Cl)OO + OH → CC(Cl)C(Cl)O[O] + H_2O	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G223☒	CC(Cl)C(Cl)OO → CC(Cl)C(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G224☒	CC(Cl)C(Cl)[O] → CC(Cl)C(=O)Cl + HO_2	k = $2.50 \cdot 10^{-14}$exp(-300/T)	
G225☒	CC(Cl)C(=O)Cl + OH → CC(Cl)(O[O])C(=O)Cl + H_2O	k = $1.08 \cdot 10^{-12}$	
G226☒	CC(Cl)C(=O)Cl → CC(Cl)O[O] + CO + Cl	J = $5.804 \cdot 10^{-06}$*cos(χ)$^{1.092}$exp(-0.377/cos(χ))	
G227☒	CC(Cl)C(O)Cl + OH → CC(Cl)C(=O)Cl + HO_2 + H_2O	k = $1.10 \cdot 10^{-12}$	
G228☒	CC(Cl)(Cl)OO + OH → CC(Cl)(Cl)O[O] + H_2O	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G229☒	CC(Cl)(Cl)OO → CC(Cl)(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G230☒	CC(Cl)(Cl)[O] → CC(=O)Cl + Cl	k = $1.00 \cdot 10^{+06}$	
G231☒	CC(O)(Cl)Cl + OH → CC(Cl)(Cl)[O] + H_2O	k = $3.07 \cdot 10^{-13}$	
G232☒	ClC(Cl)COO + OH → ClC(Cl)CO[O] + H_2O	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G233☒	ClC(Cl)COO + OH → ClC(Cl)C=O + OH + H_2O	k = $9.64 \cdot 10^{-12}$	
G234☒	ClC(Cl)COO → ClC(Cl)C[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G235☒	ClC(Cl)C[O] → ClC(Cl)C=O + HO_2	k = $2.50 \cdot 10^{-14}$exp(-300/T)	
G236☒	ClC(Cl)C=O + NO_3 → ClC(Cl)C(=O)O[O] + HNO_3	k = $1.40 \cdot 10^{-12}$exp(-1860/T)	
G237☒	ClC(Cl)C=O + OH → ClC(Cl)C(=O)O[O] + H_2O	k = $3.09 \cdot 10^{-11}$	
G238☒	ClC(Cl)C=O → [O]OC(Cl)Cl + HO_2 + CO	J = $7.914 \cdot 10^{-05}$*cos(χ)$^{0.764}$exp(-0.364/cos(χ))	
G239☒	OCC(Cl)Cl + OH → ClC(Cl)C=O + HO_2 + H_2O	k = $1.10 \cdot 10^{-12}$	
G240☒	ClCCOO + OH → ClCCO[O] + H_2O	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G241☒	ClCCOO + OH → ClCC=O + OH + H_2O	k = $1.37 \cdot 10^{-11}$	
G242☒	ClCCOO → ClCC[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G243②	ClCC[O] + O_2 → ClCC=O + HO_2	k = $2.50 \cdot 10^{-14}$exp(-300/T)	implemented from MCM
G244②	OCCCl + OH → ClCC=O + HO_2 + H_2O	k = $4.60 \cdot 10^{-12}$	
G245☒	CC(Cl)OO + OH → CC(Cl)O[O] + H_2O	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G246☒	CC(Cl)OO + OH → CC(=O)Cl + OH + H_2O	k = $9.95 \cdot 10^{-12}$	
G247☒	CC(Cl)OO → CC(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G248☒	CC(Cl)[O] + O_2 → CC=O + Cl	k = $1.00 \cdot 10^{+06}$	
G249☒	CC(O)Cl + OH → CC(=O)Cl + HO_2 + H_2O	k = $2.77 \cdot 10^{-12}$	
G250☒	CC(=O)Cl + OH → O=C(Cl)CO[O] + H_2O	k = $3.88 \cdot 10^{-14}$	
G251☒	CC(=O)Cl → CC(=O)O[O] + Cl	J = $5.804 \cdot 10^{-06}$*cos(χ)$^{1.092}$exp(-0.377/cos(χ))	
G252☒	ClC(Cl)C(Cl)(Cl)OO + OH → ClC(Cl)C(Cl)(Cl)O[O]	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G253☒	ClC(Cl)C(Cl)(Cl)OO → ClC(Cl)C(Cl)(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G254☒	$ClC(Cl)C(Cl)(Cl)[O] + O_2 \rightarrow ClC(Cl)C(=O)Cl + Cl$	$k = 1.00 \cdot 10^{+06}$	
G255☒	$ClC(Cl)C(O)(Cl)Cl + OH \rightarrow ClC(Cl)C(Cl)(Cl)[O]$	$k = 4.85 \cdot 10^{-13}$	
G256☒	$ClCC(Cl)(Cl)OO + OH \rightarrow ClCC(Cl)(Cl)O[O]$	$k = 4.03 \cdot 10^{-12}$	
G257☒	$ClCC(Cl)(Cl)OO \rightarrow ClCC(Cl)(Cl)[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G258☒	$ClCC(Cl)(Cl)[O] + O_2 \rightarrow ClCC(=O)Cl + Cl$	$k = 1.00 \cdot 10^{+06}$	
G259☒	$ClCC(O)(Cl)Cl + OH \rightarrow ClCC(Cl)(Cl)[O]$	$k = 5.77 \cdot 10^{-13}$	
G260☒	$ClCC(=O)Cl + OH \rightarrow O=C(Cl)C(Cl)O[O]$	$k = 6.26 \cdot 10^{-14}$	
G261☒	$ClCC(=O)Cl \rightarrow ClCO[O] + CO + Cl$	$J = 5.804 \cdot 10^{-06} * \cos(\chi)^{1.092} \exp(-0.377/\cos(\chi))$	
G262☒	$ClC(Cl)C(Cl)OO + OH \rightarrow ClC(Cl)C=O + OH$	$k = 1.16 \cdot 10^{-11}$	
G263☒	$ClC(Cl)C(Cl)OO + OH \rightarrow ClC(Cl)C(Cl)O[O]$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G264☒	$ClC(Cl)C(Cl)OO \rightarrow ClC(Cl)C(Cl)[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G265☒	$ClC(Cl)C(Cl)[O] \rightarrow ClC(Cl)C=O + Cl$	$k = 1.00 \cdot 10^{+06}$	
G266☒	$ClC(Cl)C(O)Cl + OH \rightarrow ClC(Cl)C(Cl)[O]$	$k = 3.66 \cdot 10^{-12}$	
G267☒	$ClC(ON(=O)=O)COO + OH \rightarrow ClC(ON(=O)=O)CO[O]$	$k = 7.22 \cdot 10^{-12}$	
G268☒	$ClC(ON(=O)=O)COO \rightarrow ClC(ON(=O)=O)C[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G269☒	$ClC(ON(=O)=O)C[O] + O_2 \rightarrow ClC(ON(=O)=O)C=O + HO_2$	$k = 2.50 \cdot 10^{-14} \exp(-300/T)$	
G270☒	$ClC(ON(=O)=O)C[O] + O_2 \rightarrow C=O + HOCl + NO_2$	$k = 7.00 \cdot 10^{-03}$	
G271☒	$ClC(ON(=O)=O)C=O + OH \rightarrow CO + O=CCl + NO_2$	$k = 7.33 \cdot 10^{-12}$	
G272☒	$ClC(ON(=O)=O)C=O \rightarrow O=CCl + CO + HO2 + NO_2$	$J = 7.549 \cdot 10^{-06} * \cos(\chi)^{1.015} \exp(-0.324/\cos(\chi))$	
G273☒	$ClC(ON(=O)=O)C=O \rightarrow O=CCl + CO + HO_2 + NO_2$	$J = 3.363 \cdot 10^{-06} * \cos(\chi)^{1.296} \exp(-0.322/\cos(\chi))$	
G274☒	$ClC(ON(=O)=O)C=O \rightarrow HO_2 + CO + O=CCl + NO_2$	$J = 2.792 \cdot 10^{-05} * \cos(\chi)^{0.805} \exp(-0.338/\cos(\chi))$	
G275☒	$OCC(Cl)ON(=O)=O + OH \rightarrow ClC(ON(=O)=O)C=O + HO_2$	$k = 1.88 \cdot 10^{-12}$	
G276☒	$OOC(Cl)CON(=O)=O + OH \rightarrow [O]OC(Cl)CON(=O)=O$	$k = 5.20 \cdot 10^{-12}$	
G277☒	$OOC(Cl)CON(=O)=O \rightarrow [O]C(Cl)CON(=O)=O + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G278☒	$[O]C(Cl)CON(=O)=O + O_2 \rightarrow O=C(Cl)CON(=O)=O + HO_2$	$k = 2.50 \cdot 10^{-14} \exp(-300/T)$	
G279☒	$[O]C(Cl)CON(=O)=O \rightarrow NO_2 + C=O + O=CCl$	$k = 7.00 \cdot 10^{-03}$	
G280☒	$OC(Cl)CON(=O)=O + OH \rightarrow OC(Cl)C=O + NO_2$	$k = 1.03 \cdot 10^{-12}$	
G281☒	$O=C(Cl)CON(=O)=O + OH \rightarrow O=C(Cl)C=O + NO_2$	$k = 3.91 \cdot 10^{-13}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G282☒	O=C(Cl)CON(=O)=O → OC(Cl)C[O] + NO_2	J = $7.549 \cdot 10^{-06}$*cos(χ)$^{1.015}$exp(-0.324/cos(χ))	
G283☒	O=C(Cl)CON(=O)=O → C=O + CO + Cl + NO_2	J = $3.363 \cdot 10^{-06}$*cos(χ)$^{1.296}$exp(-0.322/cos(χ))	
G284☒	O=C(Cl)CON(=O)=O → C=O + NO_2 + CO + Cl	J = $2.792 \cdot 10^{-05}$*cos(χ)$^{0.805}$exp(-0.338/cos(χ))	
G285☒	[O-][O+]=CCl + CO → O=CCl	k = $1.20 \cdot 10^{-15}$	
G286☒	[O-][O+]=CCl + NO → O=CCl + NO_2	k = $1.00 \cdot 10^{-14}$	
G287☒	[O-][O+]=CCl + NO_2 → O=CCl + NO_3	k = $1.00 \cdot 10^{-15}$	
G288☒	[O-][O+]=CCl + SO_2 → O=CCl + SULF	k = $7.00 \cdot 10^{-14}$	
G289☒	[O-][O+]=CCl → O=CCl + H_2O_2	k = $6.00 \cdot 10^{-18}$	
G290☒	[O-][O+]=CCl → OC(=O)Cl	k = $1.00 \cdot 10^{-17}$	
G291☒	OC(Cl)COO + OH → OC(Cl)CO[O]	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G292☒	OC(Cl)COO + OH → OC(Cl)C=O + OH	k = $6.05 \cdot 10^{-12}$	
G293☒	OC(Cl)COO → OC(Cl)C[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G294☒	OC(Cl)C[O] + O_2 → C=O + O=CCl + HO_2	k = $1.00 \cdot 10^{+06}$	
G295☒	OC(Cl)C=O + NO_3 → OC(Cl)C(=O)O[O] + HNO_3	k = $1.40 \cdot 10^{-12}$exp(-1860/T)	
G296☒	OC(Cl)C=O + OH → OC(Cl)C(=O)O[O]	k = $8.80 \cdot 10^{-12}$	
G297☒	OC(Cl)C=O → OC(Cl)C[O] + OH	J = $2.792 \cdot 10^{-05}$*cos(χ)$^{0.805}$exp(-0.338/cos(χ))	
G298☒	OCC(O)Cl + OH → OC(Cl)C=O + HO_2	k = $4.63 \cdot 10^{-12}$	
G299☒	OCC(Cl)OO + OH → OCC(Cl)O[O]	k = $1.90 \cdot 10^{-12}$exp(190/T)	
G300☒	OCC(Cl)OO + OH → OCC(=O)Cl + OH	k = $8.90 \cdot 10^{-12}$	
G301☒	OCC(Cl)OO → OCC(Cl)[O] + OH	J = $7.649 \cdot 10^{-06}$*cos(χ)$^{0.682}$exp(-0.279/cos(χ))	
G302☒	OCC(Cl)[O] → C=O + O=CCl + HO_2	k = $1.00 \cdot 10^{+06}$	
G303☒	OCC(=O)Cl + OH → O=C(Cl)C=O + HO_2	k = $2.86 \cdot 10^{-12}$	
G304☒	OCC(=O)Cl → C=O + HO_2 + Cl + CO	J = $2.792 \cdot 10^{-05}$*cos(χ)$^{0.805}$exp(-0.338/cos(χ))	
G305☒	ClC(Cl)(Cl)C(=O)O[O] + HO_2 → 0.56 ClC(Cl)(Cl)C(=O)OO + 0.44 [O]OC(Cl)(Cl)Cl + 0.44 OH	k = $5.20 \cdot 10^{-13}$exp(980/T)	
G306②	ClC(Cl)(Cl)C(=O)O[O] + NO → [O]OC(Cl)(Cl)Cl + NO_2	k = $7.50 \cdot 10^{-12}$exp(290/T)	implemented from MCM
G307②	ClC(Cl)(Cl)C(=O)O[O] + NO_2 → O=N(=O)OOC(=O)C(Cl)(Cl)Cl	TROEMCM	implemented from MCM
G308☒	ClC(Cl)(Cl)C(=O)O[O] + NO_3 [O]OC(Cl)(Cl)Cl + NO_2	k = $4.00 \cdot 10^{-12}$	
G309②	ClC(Cl)(Cl)C(=O)O[O] → [O]OC(Cl)(Cl)Cl	k = $1.00 \cdot 10^{-11}$*RO_2	implemented from MCM

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G310☒	O=C(Cl)C(=O)Cl → CO + CO + Cl + Cl	J = $5.584 \cdot 10^{-05}$*cos(χ)$^{0.805}$exp(-0.338/cos(χ))	
G311☒	ClCC(=O)O[O] + HO_2 → 0.44 ClCO[O] + 0.44 OH + 0.15 ClCC(=O)O + 0.15 O_3 + 0.41 ClCC(=O)OO	k = $5.20 \cdot 10^{-13}$exp(980/T)	
G312②	ClCC(=O)O[O] + NO → ClCO[O] + NO_2	k = $7.50 \cdot 10^{-12}$exp(290/T)	implemented from MCM
G313②	ClCC(=O)O[O] + NO_2 → ClCC(=O)OON(=O)=O	TROEMCM	implemented from MCM
G314☒	ClCC(=O)O[O] + NO_3 → ClCO[O] + NO_2	k = $4.00 \cdot 10^{-12}$	
G315②	ClCC(=O)O[O] → 0.7 ClCO[O] + 0.3 ClCC(=O)O	k = $1.00 \cdot 10^{-11}$*RO_2	implemented from MCM
G316☒	OC(Cl)(Cl)C(=O)O[O] + HO_2 → 0.56 OC(Cl)(Cl)C(=O)OO + 0.44 O=C(Cl)Cl + 0.44 HO_2 + 0.44 OH	k = $5.20 \cdot 10^{-13}$exp(980/T)	
G317☒	OC(Cl)(Cl)C(=O)O[O] + NO → O=C(Cl)Cl + HO_2 + NO_2	k = $7.50 \cdot 10^{-12}$exp(290/T)	
G318☒	OC(Cl)(Cl)C(=O)O[O] + NO_2 → O=N(=O)OOC(=O)C(O)(Cl)Cl	TROEMCM	
G319☒	OC(Cl)(Cl)C(=O)O[O] + NO_3 → O=C(Cl)Cl + HO_2 + NO_2	k = $4.00 \cdot 10^{-12}$	
G320☒	OC(Cl)(Cl)C(=O)O[O] → O=C(Cl)Cl + HO_2	k = $7.00 \cdot 10^{-12}$*RO_2	
G321☒	ClCC(Cl)C(=O)O[O] + HO_2 → 0.15 ClCC(Cl)C(=O)O + 0.15 O_3 + 0.41 ClCC(Cl)C(=O)OO + 0.44 ClCC(Cl)O[O] + 0.44 OH	k = $5.20 \cdot 10^{-13}$exp(980/T)	
G322☒	ClCC(Cl)C(=O)O[O] + NO → ClCC(Cl)O[O] + NO_2	k = $7.50 \cdot 10^{-12}$exp(290/T)	
G323☒	ClCC(Cl)C(=O)O[O] + NO_2 → ClCC(Cl)C(=O)OON(=O)=O	TROEMCM	
G324☒	ClCC(Cl)C(=O)O[O] + NO_3 → ClCC(Cl)O[O] + NO_2	k = $4.00 \cdot 10^{-12}$	
G325☒	ClCC(Cl)C(=O)O[O] → 0.3 ClCC(Cl)C(=O)O + 0.7 ClCC(Cl)O[O]	k = $1.00 \cdot 10^{-11}$*RO_2	
G326②	CC(=O)CCl + OH → CC(=O)C(Cl)O[O]	k = $3.68 \cdot 10^{-13}$	implemented from MCM
G327②	CC(=O)CCl → CO[O] + ClCC(=O)O[O]	J = $5.804 \cdot 10^{-06}$*cos(χ)$^{1.092}$exp(-0.377/cos(χ))	implemented from MCM
G328☒	CC(Cl)(O[O])C(=O)Cl + HO_2 → CC(Cl)(OO)C(=O)Cl	k = $3.30 \cdot 10^{-13}$exp(820/T)	
G329☒	CC(Cl)(O[O])C(=O)Cl + NO →	k = $2.70 \cdot 10^{-12}$exp(360/T)	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	CC(Cl)([O])C(=O)Cl + NO_2		
G330☒	CC(Cl)(O[O])C(=O)Cl + NO_3 → CC(Cl)([O])C(=O)Cl + NO_2	$k = 2.30 \cdot 10^{-12}$	
G331☒	CC(Cl)(O[O])C(=O)Cl → CC(Cl)([O])C(=O)Cl	$k = 9.20 \cdot 10^{-14} * RO_2$	
G332☒	ClC(Cl)C(=O)O[O] + HO_2 → 0.15 ClC(Cl)C(=O)O + 0.15 O_3 + 0.41 ClC(Cl)C(=O)OO + 0.44 [O]OC(Cl)Cl + 0.44 OH	$k = 5.20 \cdot 10^{-13} \exp(980/T)$	
G333☒	ClC(Cl)C(=O)O[O] + NO → [O]OC(Cl)Cl + NO_2	$k = 7.50 \cdot 10^{-12} \exp(290/T)$	
G334☒	ClC(Cl)C(=O)O[O] + NO_2 → O=N(=O)OOC(=O)C(Cl)Cl	TROEMCM	
G335☒	ClC(Cl)C(=O)O[O] + NO_3 → [O]OC(Cl)Cl + NO_2	$k = 4.00 \cdot 10^{-12}$	
G336☒	ClC(Cl)C(=O)O[O] → 0.3 ClC(Cl)C(=O)O + 0.7 [O]OC(Cl)Cl	$k = 1.00 \cdot 10^{-11} * RO_2$	
G337☒	O=C(Cl)CO[O] + HO_2 → O=C(Cl)COO	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G338☒	O=C(Cl)CO[O] + NO → O=C(Cl)C[O] + NO_2	$k = 3.24 \cdot 10^{-12} \exp(360/T)$	
G339☒	O=C(Cl)CO[O] + NO_3 → O=C(Cl)C[O] + NO_2	$k = 2.30 \cdot 10^{-12}$	
G340☒	O=C(Cl)CO[O] → O=C(Cl)C[O]	$k = 2.00 \cdot 10^{-12} * RO_2$	
G341☒	ClC(Cl)C(=O)Cl + OH → O=C(Cl)C(Cl)(Cl)O[O]	$k = 5.53 \cdot 10^{-12}$	
G342☒	ClC(Cl)C(=O)Cl → [O]OC(Cl)Cl + CO + Cl	$J = 5.804 \cdot 10^{-06} * \cos(\chi)^{1.092} \exp(-0.377/\cos(\chi))$	
G343☒	O=C(Cl)C(Cl)O[O] + HO_2 → O=C(Cl)C(Cl)OO	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G344☒	O=C(Cl)C(Cl)O[O] + NO → O=C(Cl)C(Cl)[O] + NO_2	$k = 4.05 \cdot 10^{-12} \exp(360/T)$	
G345☒	O=C(Cl)C(Cl)O[O] + NO_3 → O=C(Cl)C(Cl)[O] + NO_2	$k = 2.30 \cdot 10^{-12}$	
G346☒	O=C(Cl)C(Cl)O[O] → 0.2 OC(Cl)C(=O)Cl + 0.6 O=C(Cl)C(Cl)[O] + 0.2 O=C(Cl)C(=O)Cl	$k = 8.80 \cdot 10^{-13} * RO_2$	
G347☒	O=C(Cl)C=O + NO_3 → CO + CO + Cl + HNO_3	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	
G348☒	O=C(Cl)C=O + OH → CO + CO + Cl	$k = 1.40 \cdot 10^{-11}$	
G349☒	O=C(Cl)C=O → CO + CO + HO_2 + Cl	$J = 1.537 \cdot 10^{-04} * \cos(\chi)^{0.17} \exp(-0.208/\cos(\chi))$	
G350☒	OC(=O)Cl + OH → Cl + CO_2 + H_2O	$k = 5.20 \cdot 10^{-13}$	
G351☒	OC(Cl)C(=O)O[O] + HO_2 →	$k = 5.20 \cdot 10^{-13} \exp(980/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	0.44 O=CCl + 0.44 HO_2 + 0.15 OC(Cl)C(=O)O + 0.15 O_3 + 0.41 OC(Cl)C(=O)OO + 0.44 OH		
G352☒	OC(Cl)C(=O)O[O] + NO → O=CCl + HO_2 + NO_2	$k = 7.50 \cdot 10^{-12} \exp(290/T)$	
G353☒	OC(Cl)C(=O)O[O] + NO_2 → O=N(=O)OOC(=O)C(O)Cl	TROEMCM	
G354☒	OC(Cl)C(=O)O[O] + NO_3 → O=CCl + HO_2 + NO_2	$k = 4.00 \cdot 10^{-12}$	
G355☒	OC(Cl)C(=O)O[O] → 0.7 O=CCl + 0.7 HO_2 + 0.3 OC(Cl)C(=O)O	$k = 5.00 \cdot 10^{-12} * RO_2$	
G356☒	ClC(Cl)(Cl)C(=O)OO + OH → ClC(Cl)(Cl)C(=O)O[O]	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G357☒	ClC(Cl)(Cl)C(=O)OO → [O]OC(Cl)(Cl)Cl + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G358②	O=N(=O)OOC(=O)C(Cl)(Cl)Cl → ClC(Cl)(Cl)C(=O)O[O] + NO_2	TROEMCM	implemented from MCM
G359②	ClCC(=O)O + OH → ClCO[O]	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	implemented from MCM
G360②	ClCC(=O)OO + OH → ClCC(=O)O[O]	$k = 4.29 \cdot 10^{-12}$	
G361②	ClCC(=O)OO → ClCO[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	implemented from MCM
G362②	ClCC(=O)OON(=O)=O + OH → O=CCl + CO + NO_2	$k = 6.26 \cdot 10^{-13}$	implemented from MCM
G363②	ClCC(=O)OON(=O)=O → ClCC(=O)O[O] + NO_2	TROEMCM	implemented from MCM
G364☒	OC(Cl)(Cl)C(=O)OO + OH → OC(Cl)(Cl)C(=O)O[O]	$k = 3.59 \cdot 10^{-12}$	
G365☒	OC(Cl)(Cl)C(=O)OO → O=C(Cl)Cl + HO_2 + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G366☒	O=N(=O)OOC(=O)C(O)(Cl)Cl + OH → OC(Cl)(Cl)C(=O)O[O] + NO_2	$k = 6.00 \cdot 10^{-13}$	
G367☒	O=N(=O)OOC(=O)C(O)(Cl)Cl → OC(Cl)(Cl)C(=O)O[O] + NO_2	TROEMCM	
G368☒	ClCC(Cl)C(=O)O + OH → ClCC(Cl)O[O]	$k = 2.10 \cdot 10^{-12}$	
G369☒	ClCC(Cl)C(=O)OO + OH → ClCC(Cl)C(=O)O[O]	$k = 5.65 \cdot 10^{-12}$	
G370☒	ClCC(Cl)C(=O)OO → ClCC(Cl)O[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G371☒	ClCC(Cl)C(=O)OON(=O)=O + OH → ClCC(=O)Cl + CO + NO_2	$k = 2.42 \cdot 10^{-12}$	
G372☒	ClCC(Cl)C(=O)OON(=O)=O → ClCC(Cl)C(=O)O[O] + NO_2	TROEMCM	
G373☒	CC(=O)C(Cl)O[O] + HO_2 → CC(=O)C(Cl)OO	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G374②	CC(=O)C(Cl)O[O] + NO → CC(=O)C(Cl)[O] + NO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	implemented from MCM
G375☒	CC(=O)C(Cl)O[O] + NO_3 → CC(=O)C(Cl)[O] + NO_2	$k = 2.30 \cdot 10^{-12}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G376②	CC(=O)C(Cl)O[O] → CC(=O)C(Cl)[O]	$k = 8.80 \cdot 10^{-13} * RO_2$	implemented from MCM
G377☒	CC(Cl)(OO)C(=O)Cl + OH → CC(Cl)(O[O])C(=O)Cl	$k = 4.12 \cdot 10^{-12}$	
G378☒	CC(Cl)(OO)C(=O)Cl → CC(Cl)([O])C(=O)Cl + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G379☒	CC(Cl)([O])C(=O)Cl + O_2 → CC(=O)Cl + CO + Cl	$k = 1.00 \cdot 10^{+06}$	
G380☒	ClC(Cl)C(=O)O + OH → [O]OC(Cl)Cl	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G381☒	ClC(Cl)C(=O)OO + OH → ClC(Cl)C(=O)O[O]	$k = 3.80 \cdot 10^{-12}$	
G382☒	ClC(Cl)C(=O)OO → [O]OC(Cl)Cl + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G383☒	O=N(=O)OOC(=O)C(Cl)Cl + OH → O=C(Cl)Cl + CO + NO_2	$k = 5.70 \cdot 10^{-13}$	
G384☒	O=N(=O)OOC(=O)C(Cl)Cl → ClC(Cl)C(=O)O[O] + NO_2	TROEMCM	
G385☒	O=C(Cl)COO + OH → O=C(Cl)CO[O]	$k = 7.25 \cdot 10^{-12}$	
G386☒	O=C(Cl)COO → O=C(Cl)C[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G387☒	O=C(Cl)C[O] + O_2 → C=O + CO + Cl	$k = 1.00 \cdot 10^{+06}$	
G388☒	O=C(Cl)C(Cl)(Cl)O[O] + HO_2 → O=C(Cl)C(Cl)(Cl)OO	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G389☒	O=C(Cl)C(Cl)(Cl)O[O] + NO → O=C(Cl)C(Cl)(Cl)[O] + NO_2	$k = 4.05 \cdot 10^{-12} \exp(360/T)$	
G390☒	O=C(Cl)C(Cl)(Cl)O[O] + NO_3 → O=C(Cl)C(Cl)(Cl)[O] + NO_2	$k = 2.30 \cdot 10^{-12}$	
G391☒	O=C(Cl)C(Cl)(Cl)O[O] → 0.3 OC(Cl)(Cl)C(=O)Cl + 0.7 O=C(Cl)C(Cl)(Cl)[O]	$k = 9.20 \cdot 10^{-14} * RO_2$	
G392☒	O=C(Cl)C(Cl)OO + OH → O=C(Cl)C(Cl)O[O]	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G393☒	O=C(Cl)C(Cl)OO + OH → O=C(Cl)C(=O)Cl + OH	$k = 4.00 \cdot 10^{-12}$	
G394☒	O=C(Cl)C(Cl)OO → O=C(Cl)C(Cl)[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G395☒	O=C(Cl)C(Cl)[O] → O=CCl + CO + Cl	$k = 1.00 \cdot 10^{+06}$	
G396☒	OC(Cl)C(=O)O + OH → O=CCl + HO_2	$k = 2.57 \cdot 10^{-12}$	
G397☒	OC(Cl)C(=O)OO + OH → OC(Cl)C(=O)O[O]	$k = 5.67 \cdot 10^{-12}$	
G398☒	OC(Cl)C(=O)OO → O=CCl + HO_2 + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G399☒	O=N(=O)OOC(=O)C(O)Cl + OH → O=CCl + CO + NO_2	$k = 2.08 \cdot 10^{-12}$	
G400☒	O=N(=O)OOC(=O)C(O)Cl → OC(Cl)C(=O)O[O] + NO_2	TROEMCM	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G401☒	CC(=O)C(Cl)OO + OH → CC(=O)C(Cl)O[O]	$k = 8.34 \cdot 10^{-12}$	
G402☒	CC(=O)C(Cl)OO → CC(=O)C(Cl)[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G403☒	CC(=O)C(Cl)[O] + O_2 → O=CCl + CC(=O)O[O]	$k = 1.00 \cdot 10^{+06}$	
G404☒	O=C(Cl)C(Cl)(Cl)OO + OH → O=C(Cl)C(Cl)(Cl)O[O]	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G405☒	O=C(Cl)C(Cl)(Cl)OO → O=C(Cl)C(Cl)(Cl)[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G406☒	O=C(Cl)C(Cl)(Cl)[O] → O=C(Cl)C(=O)Cl + Cl	$k = 1.00 \cdot 10^{+06}$	
G407②	Cl_2 → Cl + Cl	$J = 3.827 \cdot 10^{-03} * \cos(\chi)^{0.543} \exp(-0.244/\cos(\chi))$	
G408②	ClO → Cl + O^3PX	$J = 4.755 \cdot 10^{-04} * \cos(\chi)^{1.258} \exp(-0.588/\cos(\chi))$	
G409②	OClO → ClO + O^3PX	$J = 1.332 \cdot 10^{-01} * \cos(\chi)^{0.416} \exp(-0.244/\cos(\chi))$	
G410②	Cl_2O_2 → Cl + ClO_2	$J = 2.294 \cdot 10^{-03} * \cos(\chi)^{0.745} \exp(-0.223/\cos(\chi))$	
G411②	Cl_2O_3 → ClO + OClO	$J = 1.558 \cdot 10^{-03} * \cos(\chi)^{1.324} \exp(-0.462/\cos(\chi))$	
G412②	HOCl → Cl + OH	$J = 4.615 \cdot 10^{-04} * \cos(\chi)^{0.656} \exp(-0.240/\cos(\chi))$	
G413②	ClNO → Cl + NO	$J = 4.755 \cdot 10^{-03} * \cos(\chi)^{0.408} \exp(-0.217/\cos(\chi))$	
G414②	$ClNO_2$ → Cl + NO_2	$J = 6.219 \cdot 10^{-04} * \cos(\chi)^{0.774} \exp(-0.255/\cos(\chi))$	
G415②	$ClNO_3$ → Cl + NO_3	$J = 6.420 \cdot 10^{-05} * \cos(\chi)^{0.648} \exp(-0.217/\cos(\chi))$	
G416②	$ClNO_3$ → ClO + NO_2	$J = 1.393 \cdot 10^{-05} * \cos(\chi)^{1.052} \exp(-0.243/\cos(\chi))$	
G417②	CC(=O)C(=O)Cl → O=[C]Cl + CC(=O)O[O]	$J = 1.853 \cdot 10^{-04} * \cos(\chi)^{0.583} \exp(-0.225/\cos(\chi))$	
G418②	ClCC(=O)O → ClC[O] + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G419②	Br_2 → Br + Br	$J = 4.773 \cdot 10^{-02} * \cos(\chi)^{0.193} \exp(-0.213/\cos(\chi))$	
G420②	BrO → Br + O^3PX	$J = 6.368 \cdot 10^{-02} * \cos(\chi)^{0.605} \exp(-0.269/\cos(\chi))$	
G421②	OBrO → BrO + O^3PX	$J = 6.880 \cdot 10^{-01} * \cos(\chi)^{0.144} \exp(-0.198/\cos(\chi))$	
G422②	HOBr → Br + OH	$J = 3.464 \cdot 10^{-03} * \cos(\chi)^{0.441} \exp(-0.214/\cos(\chi))$	
G423②	$BrNO_2$ → Br + NO_2	$J = 7.443 \cdot 10^{-03} * \cos(\chi)^{0.355} \exp(-0.236/\cos(\chi))$	
G424②	$BrNO_3$ → Br + NO_3	$J = 6.363 \cdot 10^{-04} * \cos(\chi)^{0.492} \exp(-0.215/\cos(\chi))$	
G425②	$BrNO_3$ → BrO + NO_2	$J = 1.558 \cdot 10^{-03} * \cos(\chi)^{0.490} \exp(-0.216/\cos(\chi))$	
G426②	BrCl → Br + Cl	$J = 1.650 \cdot 10^{-02} * \cos(\chi)^{0.297} \exp(-0.224/\cos(\chi))$	
G427②	CC(=O)CBr → 0.7 O=[C]Br + 0.7 CC(=O)O[O] + 0.3 BrCC(=O)O[O] + 0.3 CO[O]	$J = 3.523 \cdot 10^{-04} * \cos(\chi)^{0.885} \exp(-0.283/\cos(\chi))$	
G428②	CC(=O)C(=O)Br → O=[C]Br + CC(=O)O[O]	$J = 1.853 \cdot 10^{-04} * \cos(\chi)^{0.583} \exp(-0.225/\cos(\chi))$	
G429②	BrC(Br)Br → Br + BrC(Br)O[O]	$J = 2.228 \cdot 10^{-06} * \cos(\chi)^{1.471} \exp(-0.230/\cos(\chi))$	
G430②	BrCBr → Br + BrCO[O]	$J = 5.600 \cdot 10^{-09} * \cos(\chi)^{2.763} \exp(-1.922/\cos(\chi))$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G431②	O=C(Br)Br → 2.0 Br + CO	$J = 4.377 \cdot 10^{-06} * \cos(\chi)^{1.360} \exp(-0.273/\cos(\chi))$	
G432②	I_2 → I + I	$J = 2.165 \cdot 10^{-01} * \cos(\chi)^{0.125} \exp(-0.185/\cos(\chi))$	
G433②	IO → I + O^3PX	$J = 2.640 \cdot 10^{-03} * \cos(\chi)^{0.240} \exp(-0.240/\cos(\chi))$	
G434②	OIO → I	$J = 4.054 \cdot 10^{-02} * \cos(\chi)^{0.119} \exp(-0.185/\cos(\chi))$	
G435②	OIO → IO + O^3PX	$J = 1.894 \cdot 10^{-03} * \cos(\chi)^{0.119} \exp(-0.185/\cos(\chi))$	
G436②	I_2O_2 → 2.0 I	$J = 2.294 \cdot 10^{-03} * \cos(\chi)^{0.745} \exp(-0.223/\cos(\chi))$	
G437②	HI → I + HO_2	$J = 2.104 \cdot 10^{-04} * \cos(\chi)^{1.123} \exp(-0.281/\cos(\chi))$	
G438②	HOI → I + OH	$J = 1.469 \cdot 10^{-02} * \cos(\chi)^{0.342} \exp(-0.236/\cos(\chi))$	
G439②	INO → I + NO	$J = 4.849 \cdot 10^{-02} * \cos(\chi)^{0.284} \exp(-0.232/\cos(\chi))$	
G440②	INO_2 → I + NO_2	$J = 5.036 \cdot 10^{-03} * \cos(\chi)^{0.568} \exp(-0.256/\cos(\chi))$	
G441②	INO_3 → I + NO_3	$J = 6.599 \cdot 10^{-02} * \cos(\chi)^{0.530} \exp(-0.243/\cos(\chi))$	
G442②	INO_3 → IO + NO_2	$J = 1.165 \cdot 10^{-02} * \cos(\chi)^{0.528} \exp(-0.244/\cos(\chi))$	
G443②	ICl → I + Cl	$J = 3.403 \cdot 10^{-02} * \cos(\chi)^{0.179} \exp(-0.207/\cos(\chi))$	
G444②	IBr → I + Br	$J = 1.000 \cdot 10^{-01} * \cos(\chi)^{0.149} \exp(-0.197/\cos(\chi))$	
G445②	CC(I)C → I + CC(O[O])C	$J = 3.731 \cdot 10^{-05} * \cos(\chi)^{1.292} \exp(-0.217/\cos(\chi))$	
G446②	ICC → I + CCO[O]	$J = 1.386 \cdot 10^{-05} * \cos(\chi)^{1.324} \exp(-0.224/\cos(\chi))$	
G447②	ICC=O → [O]OCI + CO + HO_2	$J = 4.642 \cdot 10^{-05} * \cos(\chi)^{0.762} \exp(-0.353/\cos(\chi))$	
G448②	ICC(=O)OO → [O]OCI + CO_2 + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G449②	ICI → I + [O]OCI	$J = 1.496 \cdot 10^{-02} * \cos(\chi)^{0.801} \exp(-0.265/\cos(\chi))$	
G450②	CI → I + CO[O]	$J = 1.206 \cdot 10^{-05} * \cos(\chi)^{1.254} \exp(-0.231/\cos(\chi))$	
G451②	OOCI → [O]CI + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G452②	O=CI → I + CO + HO_2	$J = 2.547 \cdot 10^{-05} * \cos(\chi)^{1.393} \exp(-0.361/\cos(\chi))$	
G453②	ClCI → I + ClCO[O]	$J = 6.910 \cdot 10^{-04} * \cos(\chi)^{1.057} \exp(-0.238/\cos(\chi))$	
G454②	BrCI → I + BrCO[O]	$J = 4.261 \cdot 10^{-04} * \cos(\chi)^{0.976} \exp(-0.250/\cos(\chi))$	
G455②	Cl + O_3 → ClO	$k = 2.80 \cdot 10^{-11} \exp(-250/T)$	
G456②	Cl + H_2 → HCl + HO_2	$k = 3.90 \cdot 10^{-11} \exp(-2310/T)$	
G457⦸	Cl + HO_2 → HCl	$k = 3.48 \cdot 10^{-11}$	revised after IUPAC
G458⦸	Cl + HO_2 → ClO + OH	$k = 7.48 \cdot 10^{-11} \exp(-620/T)$	revised after IUPAC
G459②	Cl + H_2O_2 → HCl + HO_2	$k = 1.10 \cdot 10^{-11} \exp(-980/T)$	
G460②	Cl_2 + OH → HOCl + Cl	$k = 3.60 \cdot 10^{-12} \exp(-1200/T)$	
G461②	ClO + O_3 → ClO_2	$k = 2.00 \cdot 10^{-12} \exp(-3600/T)$	
G462②	ClO + O_3 → OClO	$k = 1.00 \cdot 10^{-12} \exp(-4000/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G463②	$ClO + OH \rightarrow 0.94\ HO_2 + 0.94\ Cl + 0.06\ HCl$	$k = 7.30 \cdot 10^{-12} \exp(300/T)$	
G464②	$ClO + HO_2 \rightarrow HOCl$	$k = 2.20 \cdot 10^{-12} \exp(340/T)$	
G465②	$ClO + ClO \rightarrow Cl_2$	$k = 1.00 \cdot 10^{-12} \exp(-1590/T)$	
G466②	$ClO + ClO \rightarrow Cl + ClO_2$	$k = 3.00 \cdot 10^{-11} \exp(-2450/T)$	
G467②	$ClO + ClO \rightarrow Cl + OClO$	$k = 3.50 \cdot 10^{-13} \exp(-1370/T)$	
G468⦸	$ClO + ClO \rightarrow Cl_2O_2$	TROE	[1]
G469②	$Cl + O_2 \rightarrow ClO_2$	TROE	
G470②	$ClO_2 \rightarrow Cl$	$k = 2.80 \cdot 10^{-10} \exp(-1820/T)$	
G471②	$Cl + ClO_2 \rightarrow 0.1\ ClO + 0.95\ Cl_2$	$k = 2.42 \cdot 10^{-10}$	
G472②	$Cl_2O_2 \rightarrow ClO + ClO$	TROEXP	
G473②	$Cl_2O_2 + O_3 \rightarrow ClO + ClO_2$	$k = 1.00 \cdot 10^{-19}$	
G474②	$Cl_2O_2 + Cl \rightarrow Cl_2 + ClO_2$	$k = 7.60 \cdot 10^{-11} \exp(65/T)$	
G475②	$OClO + OH \rightarrow HOCl$	$k = 1.40 \cdot 10^{-12} \exp(600/T)$	
G476②	$OClO + Cl \rightarrow ClO + ClO$	$k = 3.20 \cdot 10^{-11} \exp(170/T)$	
G477②	$OClO + ClO \rightarrow Cl_2O_3$	TROE	
G478②	$Cl_2O_3 \rightarrow OClO + ClO$	TROEXP	
G479②	$HCl + OH \rightarrow Cl$	$k = 1.70 \cdot 10^{-12} \exp(-230/T)$	
G480②	$HOCl + OH \rightarrow ClO$	$k = 3.00 \cdot 10^{-12} \exp(-500/T)$	
G481⦸	$HOCl + Cl \rightarrow 0.76\ HCl + 0.76\ ClO + 0.24\ Cl_2 + 0.24\ OH$	$k = 3.40 \cdot 10^{-12} \exp(-130/T)$	[1]
G482②	$ClO + NO \rightarrow Cl + NO_2$	$k = 6.20 \cdot 10^{-12} \exp(295/T)$	
G483②	$OClO + NO \rightarrow ClO + NO_2$	$k = 1.10 \cdot 10^{-13} \exp(350/T)$	
G484②	$Cl + NO_3 \rightarrow ClO + NO_2$	$k = 2.40 \cdot 10^{-11}$	
G485②	$ClO + NO_3 \rightarrow 0.68\ ClO_2 + 0.32\ OClO + NO_2$	$k = 4.61 \cdot 10^{-13}$	
G486②	$Cl + NO \rightarrow ClNO$	$k = [M] * 7.60 \cdot 10^{-32} (T/300)^{1.8}$	
G487②	$Cl + ClNO \rightarrow Cl_2 + NO$	$k = 5.80 \cdot 10^{-11} \exp(100/T)$	
G488②	$Cl + NO_2 \rightarrow ClNO_2$	TROE	
G489②	$ClNO_2 + OH \rightarrow HOCl + NO_2$	$k = 2.40 \cdot 10^{-12} \exp(-1250/T)$	
G490②	$ClO + NO_2 \rightarrow ClNO_3$	TROEF	
G491②	$ClNO_3 \rightarrow ClO + NO_2$	$k = [M] * 2.75 \cdot 10^{-6} \exp(11438/T)$	
G492②	$ClNO_3 + OH \rightarrow 0.5\ HOCl + 0.5\ NO_3 + 0.5\ ClO + 0.5\ HNO_3$	$k = 1.20 \cdot 10^{-12} \exp(-330/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G493②	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	$k = 6.20 \cdot 10^{-12} \exp(145/T)$	
G494⦸	$Cl + OC \rightarrow C{=}O + HO_2 + HCl$	$k = 7.10 \cdot 10^{-11} \exp(-75/T)$	revised after IUPAC
G495⦸	$Cl + CCO \rightarrow$ 0.92 $CC{=}O + 0.92\ HO_2 + 0.08\ OCCO[O] + HCl$	$k = 6.05 \cdot 10^{-11} \exp(155/T)$	revised after IUPAC
G496⦸	$Cl + CCCO \rightarrow$ 0.6 $CCC{=}O + 0.6\ HO_2 + 0.15\ OCCCO[O]$ + 0.25 $CC(O[O])CO + HCl$	$k = 2.70 \cdot 10^{-11} \exp(525/T)$	revised after IUPAC
G497⦸	$Cl + CC(O)C \rightarrow$ 0.85 $CC(=O)C + 0.85\ HO_2 + 0.15\ CC(O)CO[O] + HCl$	$k = 8.70 \cdot 10^{-11}$	revised after IUPAC
G498②	$Cl + CCCCO \rightarrow$ 0.358 $CCCC{=}O + 0.358\ HO_2 + 0.321\ CCC(O[O])CO$ + 0.321 $CC(O[O])CCO + HCl$	$k = 3.50 \cdot 10^{-11} \exp(550/T)$	
G499	$Cl + CCC(O)C \rightarrow$ $HCl + 0.361\ CC(O)C(O[O])C + 0.639\ CCC(=O)C$ + 0.639 HO_2	$k = 6.16 \cdot 10^{-11} \exp(174/T)$	[2], products MCM
G500	$Cl + CC(C)CO \rightarrow$ $HCl + 0.558\ CC(O[O])(C)CO + 0.090\ CC(CO)CO[O]$ + 0.352 $CC(C)C{=}O + 0.352\ HO_2$	$k = 1.89 \cdot 10^{-10}$	[3], mean of two relative rate constants, products MCM
G501	$Cl + CC(O)(C)C \rightarrow$ $HCl + 0.888\ CC(O)(C)CO[O] + 0.112\ CC([O])(C)C$	$k = 3.28 \cdot 10^{-11}$	[3], mean of two relative rate constants, products MCM
G502	$Cl + CCCCCO \rightarrow HCl + CCCCC{=}O + HO_2$	$k = 4.49 \cdot 10^{-11} \exp(533/T)$	Rate constant mean from [4], [3], [5]& [6], product MCM
G503	$Cl + CCCC(O)C \rightarrow HCl + CCCC(=O)C + HO_2$	$k = 2.10 \cdot 10^{-10}$	[4]
G504	$Cl + CCC(O)CC \rightarrow$ $HCl + 0.436\ CCC(=O)CC + 0.436\ HO_2$ + 0.07 $CCC(O)CCO[O] + 0.493\ CCC(O)C(O[O])C$	$k = 2.03 \cdot 10^{-10}$	[7], only measurement
G505	$Cl + CCC(C)CO \rightarrow$ $HCl + 0.288\ CCC(C)C{=}O + 0.288\ HO_2$ + 0.258 $CC(O[O])C(C)CO + 0.454\ CCC(O[O])(C)CO$	$k = 1.91 \cdot 10^{-10}$	[8]
G506	$Cl + CC(C)CCO \rightarrow$ $HCl + 0.288\ CC(C)CC{=}O + 0.288\ HO_2$ + 0.454 $CC(O[O])(C)CCO + 0.258\ CC(C)C(O[O])CO$	$k = 2.36 \cdot 10^{-10}$	[3], mean of two relative rate constants, products MCM
G507	$Cl + CCC(O)(C)C \rightarrow$	$k = 2.48 \cdot 10^{-11} \exp(328/T)$	[2], products after MCM

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	HCl + 0.100 CC(O)(C)CCO[O] + 0.701 CC(O[O])C(O)(C)C + 0.199 CCC(O)(C)CO[O]		
G508	Cl + CC(O)C(C)C → HCl + 0.074 CC(O)C(C)CO[O] + 0.463 CC(=O)C(C)C + 0.463 CC(O)C(O[O])(C)C + 0.463 HO_2	$k = 6.29 \cdot 10^{-11} \exp(192/T)$	[2], products after MCM
G509	Cl + CCCCCCO → HCl + CCCCCC=O + HO_2	$k = 2.95 \cdot 10^{-10}$	[5], products after MCM
G510	Cl + CC(O)(C)C(C)C → HCl + CC([O])(C)C(C)C	$k = 4.80 \cdot 10^{-11} \exp(221/T)$	[2], products after MCM
G511	Cl + C1CCC(O)CC1 → HCl + 0.739 C1CC(O)C(O[O])CC1 + 0.261 C1CCC(=O)CC1 + 0.261 HO_2	$k = 2.99 \cdot 10^{-10}$	[8]
G512	Cl + CC(=O)CC(O)(C)C → HCl + 0.693 CC(=O)C(O[O])C(O)(C)C + 0.270 CC(=O)CC(O)(C)CO[O] + 0.037 CC(O)(C)CC(=O)CO[O]	$k = 4.88 \cdot 10^{-11}$	[8]
G513	Cl + OCCO → HCl + OCC=O + HO_2	$k = 2.50 \cdot 10^{-10}$	[8]
G514	Cl + CC(O)CO → HCl + 0.613 CC(=O)CO + 0.613 HO_2 + 0.387 CC(O)C=O + 0.387 HO_2	$k = 2.054 \cdot 10^{-10}$	[8]
G515⦸	Cl + COO → HCl + 0.6 CO[O] + 0.4 C=O + 0.4 OH	$k = 5.90 \cdot 10^{-11}$	revised after IUPAC
G516	Cl + CCOO → HCl + CC=O + OH	$k = 1.07 \cdot 10^{-10}$	[9], products [10]
G517②	Cl + CO[O] → 0.5 C=O + 0.5 ClO + 0.5 HO2 + 0.5 HCl + 0.5 O=CO	$k = 1.60 \cdot 10^{-10}$	
G518②	Cl + O=CO → HO_2 + HCl	$k = 1.90 \cdot 10^{-13}$	
G519②	Cl + CC(=O)O → CO[O] + HCl	$k = 2.65 \cdot 10^{-14}$	
G520⦸	ClO + CO[O] → ClO_2 + C=O + HO_2	$k = 1.80 \cdot 10^{-11} \exp(-600/T)$	revised after [1]
G521⦸	Cl + C=O → HCl + CO + HO_2	$k = 8.10 \cdot 10^{-11} \exp(-34/T)$	revised after IUPAC
G522②	ClO + C=O → HOCl + CO + HO_2	$k = 1.00 \cdot 10^{-12} \exp(-2100/T)$	
G523②	Cl + CC=O → HCl + 0.99 CC(=O)O[O] + 0.01 O=CCO[O]	$k = 8.00 \cdot 10^{-11}$	
G524②	Cl + CCC=O → HCl + CCC(=O)O[O]	$k = 1.30 \cdot 10^{-10}$	
G525	Cl + CCCC=O → HCl + 0.34 CC(O[O])CC=O + 0.66 CCCC(=O)O[O]	$k = 1.63 \cdot 10^{-10}$	[11], products after MCM
G526	Cl + CC(C)C=O →	$k = 1.70 \cdot 10^{-10}$	[12], products [13]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	HCl + 0.12 CC(C=O)CO[O] + 0.03 CC(O[O])(C)C=O + 0.85 CC(C)C(=O)O[O]		
G527	Cl + CCCCC=O → HCl + 0.55 CCC(O[O])CC=O + 0.45 CCCCC(=O)O[O]	$k = 2.56 \cdot 10^{-10}$	[14], products MCM, yields [11]
G528	Cl + CC(C)(C)C=O → HCl + CC(C)(C)C(=O)O[O]	$k = 1.20 \cdot 10^{-10}$	[15], products after MCM
G529	Cl + CCCCCC=O → HCl + CCCCCC(=O)O[O]	$k = 2.88 \cdot 10^{-10}$	[14]
G530	Cl + CCCCCCC=O → HCl + CCCCCCC(=O)O[O]	$k = 3.00 \cdot 10^{-10}$	[14]
G531②	Cl + CC(=O)C=O → HCl + CC(=O)C(=O)O[O]	$k = 4.80 \cdot 10^{-11}$	
G532②	Cl + O=CC=O → HCl + 2.0 CO + HO_2	$k = 3.80 \cdot 10^{-11}$	
G533	Cl + O=CC=CC=O → O=CC=CC(=O)O[O] + HCl	$k = 1.35 \cdot 10^{-10}$	[16], products NO_3 reaction
G534	Cl + O=CC=C → 0.22 HCl + 0.22 C=CC(=O)O[O] + 0.78 ClCC(O[O])C=O	$k = 2.20 \cdot 10^{-10}$	[17]
G535	ClCC(O[O])C=O + HO_2 → ClCC(OO)C=O	$k = 1.51 \cdot 10^{-13} \exp(1300/T)$	after MCM
G536	ClCC(O[O])C=O + NO → ClCC=O + HO_2 + CO + NO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	Rate constant MCM, products [17]
G537	ClCC(O[O])C=O + NO_3 → ClCC=O + HO_2 + CO + NO_2	$k = 2.30 \cdot 10^{-12}$	Rate constant MCM, products[17]
G538	ClCC(O[O])C=O → ClCC=O + HO_2 + CO	$k = 8.80 \cdot 10^{-13} * RO_2$	Rate constant MCM, products [17]
G539	ClCC(OO)C=O + OH → ClCC(=O)C=O + OH	$k = 4.77 \cdot 10^{-11}$	after MCM
G540	ClCC(OO)C=O → ClCC=O + HO_2 + CO + OH	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	after MCM
G541	Cl + CC(C=O)=C → 0.2 C=C(C)C(=O)O[O] + 0.8 CC(O[O])(CCl)C=O + 0.2 HCl	$k = 2.55 \cdot 10^{-10}$	Rate constant average [17], [18], [19] & [20], Branching ratios [21] (consistent [22])
G542	CC(O[O])(CCl)C=O + HO_2 → 0.8 CC(OO)(CCl)C=O + 0.2 CC(=O)CCl + 0.2 CO + 0.2 HO2 + 0.2 OH	$k = 1.00 \cdot 10^{-11}$	[21], decay of RO [19]
G543	CC(O[O])(CCl)C=O + NO → CC(=O)CCl + CO + HO_2 + NO_2	$k = 1.17 \cdot 10^{-11}$	[23], decay of RO [19]
G544	CC(O[O])(CCl)C=O →	$k = 2.40 \cdot 10^{-12} * RO_2$	[21], decay of RO [19]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	CC(=O)CCl + CO + HO_2		
G545	CC(OO)(CCl)C=O → CC(=O)CCl + CO + HO_2 + OH	J = $7.914 \cdot 10^{-05} * \cos(\chi)^{0.764} \exp(-0.364/\cos(\chi))$	after MACROOH in MCM
G546	OH + CC(OO)(CCl)C=O → CC(=O)CCl + CO + OH	k = $3.77 \cdot 10^{-11}$	after MACROOH in MCM
G547	Cl + CC(=O)C=C → CC(=O)C(O[O])=CCl	k = $2.10 \cdot 10^{-10}$	[17]
G548	CC(=O)C(O[O])CCl + HO_2 → CC(=O)C(OO)CCl	k = $1.82 \cdot 10^{-13} \exp(1300/T)$	after MCM, products [17]
G549	CC(=O)C(O[O])CCl+ NO → ClCC=O + NO_2 + CC(=O)O[O]	k = $2.70 \cdot 10^{-12} \exp(360/T)$	after MCM, products [17]
G550	CC(=O)C(O[O])CCl+ NO_3 → ClCC=O + NO_2 + CC(=O)O[O]	k = $2.30 \cdot 10^{-12}$	after MCM, products [17]
G551	CC(=O)C(O[O])CCl → ClCC=O + CC(=O)O[O]	k = $8.80 \cdot 10^{-13} * RO_2$	after MCM, products [17]
G552	CC(=O)C(OO)CCl → ClCC=O + CC(=O)O[O] + OH	J = $7.649 \cdot 10^{-05} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	after MVKOOH in MCM
G553	OH + CC(=O)C(OO)CCl → ClCC=O + CC(=O)O[O] + OH	k = $3.95 \cdot 10^{-11}$	after MVKOOH in MCM
G554②	Cl + CC(=O)C → HCl + CC(=O)CO[O]	k = $3.20 \cdot 10^{-11} \exp(-815/T)$	
G555⦸	Cl + CCC(=O)C → HCl + 0.22 CC(=O)CCO[O] + 0.75 CC(=O)C(O[O])C + 0.03 CCC(=O)CO[O]	k = $3.05 \cdot 10^{-11} \exp(80/T)$	revised after IUPAC, products after [24]
G556	Cl + CCCC(=O)C → 0.82 CC(=O)CC(O[O])C + 0.18 CCC(O[O])C(=O)C + HCl	k = $1.11 \cdot 10^{-10}$	[25]
G557	Cl + CCC(=O)CC → 0.79 CCC(=O)C(O[O])C + 0.21 CCC(=O)CCO[O] + HCl	k = $5.66 \cdot 10^{-11} \exp(87/T)$	[26], products [20]
G558	Cl + CC(=O)C(C)C → HCl + 0.523 CC(=O)C(O[O])(C)C + 0.477 CC(=O)C(C)CO[O]	k = $6.80 \cdot 10^{-11}$	[27], products after MCM
G559	Cl + CCCCC(=O)C →	k = $1.88 \cdot 10^{-10}$	[25], products after MCM

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	HCl + 0.715 CC(=O)CC(O[O])CC + 0.162 CC(=O)CCC(O[O])C + 0.123 CCCC(O[O])C(=O)C		
G560	Cl + CCCC(=O)CC →	$k = 1.43 \cdot 10^{-10}$	[25], products after MCM
	HCl + 0.638 CCC(=O)CC(O[O])C + 0.142 CCC(=O)C(O[O])CC + 0.110 CCCC(=O)C(O[O])C + 0.110 CCCC(=O)CCO[O]		
G561	Cl + CC(=O)CC(C)C →	$k = 1.10 \cdot 10^{-10}$	[27], products after MCM
	HCl + 0.91 CC(=O)CC(O[O])(C)C + 0.09 CC(=O)C(O[O])C(C)C		
G562	Cl + CC(=O)C(C)(C)C →	$k = 4.80 \cdot 10^{-11}$	[27], products after MCM
	HCl + CC(=O)C(C)(C)CO[O]		
G563	Cl + CC(=O)CCC(C)C →	$k = 1.65 \cdot 10^{-10}$	[27], products after MCM
	HCl + CC(=O)CC(O[O])C(C)C		
G564	Cl + CCC(C)C(=O)C →	$k = 9.40 \cdot 10^{-11}$	[27], products after MCM
	HCl + 0.671 CC(O[O])C(C)C(=O)C + 0.329 CCC(O[O])(C)C(=O)C		
G565	Cl + C1CCC(=O)CC1 →	$k = 1.30 \cdot 10^{-10}$	[8]
	HCl + C1C(=O)CC(O[O])CC1		
G566	Cl + CC(=O)CCl → HCl + CC(=O)C(Cl)O[O]	$k = 3.50 \cdot 10^{-12}$	[28]
G567	Cl + CC(=O)C(=O)C → HCl + CC(=O)C(=O)CO[O]	$k = 2.55 \cdot 10^{-11} \exp(-1156/T)$	[29]
G568②	Cl + CC(=O)CO → HCl + CC(=O)C=O + HO_2	$k = 5.70 \cdot 10^{-11}$	
G569②	Cl + OCC=O → HCl + OCC(=O)O[O]	$k = 7.00 \cdot 10^{-11}$	
G570⦸	Cl + C#C → 0.26 O=CCl + 0.21 Cl + 0.53 HCl + 0.21 O=CC=O + 1.32 CO + 0.79 HO_2	TROE	[1]
G571②	Cl + CON(=O)=O → C=O + NO_2 + HCl	$k = 2.40 \cdot 10^{-13}$	
G572②	Cl + CCON(=O)=O → CC=O + NO_2 + HCl	$k = 4.70 \cdot 10^{-12}$	
G573②	Cl + CCCON(=O)=O → CCC=O + NO_2 + HCl	$k = 2.20 \cdot 10^{-11}$	
G574②	Cl + CC(ON(=O)=O)C → CC(=O)C + NO_2 + HCl	$k = 3.80 \cdot 10^{-12}$	
G575②	Cl + CCCCON(=O)=O → CCCC=O + NO_2 + HCl	$k = 8.50 \cdot 10^{-11}$	
G576	Cl + c1ccccc1C → HCl + c1ccccc1CO[O]	$k = 6.20 \cdot 10^{-11}$	average [30]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G577	Cl + Cc1ccccc1C → HCl + Cc1ccccc1CO[O]	$k = 1.40 \cdot 10^{-10}$	average [30]
G578	Cl + c1c(C)cccc1C → Cc1cccc(c1)CO[O] + HCl	$k = 1.35 \cdot 10^{-10}$	average [30]
G579	Cl + c1cc(C)ccc1C → Cc1ccc(CO[O])cc1 + HCl	$k = 1.44 \cdot 10^{-10}$	average [30]
G580	Cl + c1ccccc1C=O → HCl + c1ccccc1C(=O)O[O]	$k = 1.00 \cdot 10^{-10}$	[31]
G581	Cl + Cc1ccccc1C=O → HCl + Cc1ccccc1C(=O)O[O]	$k = 1.90 \cdot 10^{-10}$	[31]
G582	Cl + Cc1cccc(c1)C=O → HCl + Cc1cccc(c1)C(=O)O[O]	$k = 1.70 \cdot 10^{-10}$	[31]
G583	Cl + Cc1ccc(C=O)cc1 → HCl + Cc1ccc(C(=O)O[O])cc1	$k = 1.40 \cdot 10^{-10}$	[31]
G584	Cl + c1c(C)cc(C=O)cc1C → HCl + c1c(C)cc(C(=O)O[O])cc1C	$k = 9.60 \cdot 10^{-11}$	[32]
G585	Cl + c1ccccc1CC → c1ccccc1CCO[O] + HCl	$k = 9.10 \cdot 10^{-11}$	[8]
G586	Cl + c1ccccc1CCC → c1ccccc1C(O[O])CC + HCl	$k = 7.50 \cdot 10^{-11}$	[8]
G587	Cl + c1ccccc1C(C)C → c1ccccc1C(O[O])(C)C + HCl	$k = 8.20 \cdot 10^{-11}$	[8]
G588	Cl + Cc1cccc(C)c1C → Cc1cccc(CO[O])c1C + HCl	$k = 3.60 \cdot 10^{-10}$	[8]
G589	Cl + Cc1ccc(C)cc1C → Cc1ccc(CO[O])cc1C + HCl	$k = 3.60 \cdot 10^{-10}$	[8]
G590	Cl + c1c(C)cc(C)cc1C → c1c(C)cc(CO[O])cc1C + HCl	$k = 2.42 \cdot 10^{-10}$	[30]
G591	Cl + Cc1ccccc1CC → Cc1ccccc1C(O[O])C + HCl	$k = 1.10 \cdot 10^{-10}$	[8]
G592	Cl + c1c(C)cccc1CC → Cc1ccccc1C(O[O])C + HCl	$k = 1.40 \cdot 10^{-10}$	[8]
G593	Cl + c1cc(C)ccc1CC → Cc1ccccc1C(O[O])C + HCl	$k = 2.20 \cdot 10^{-10}$	[8]
G594	Cl + c1ccccc1C=C → c1ccccc1C(Cl)CO[O]	$k = 3.60 \cdot 10^{-10}$	[33]
G595	c1ccccc1C(Cl)CO[O] + NO → c1ccccc1C(Cl)C[O] + NO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	after OH reaction in MCM
G596	c1ccccc1C(Cl)CO[O] → c1ccccc1C(Cl)C[O]	$k = 2.50 \cdot 10^{-13}$	after OH reaction in MCM
G597	c1ccccc1C(Cl)C[O] → ClO + C=O + c1ccccc1C=O	$k = 1.00 \cdot 10^{+06}$	after OH reaction in MCM
G598	Cl + c1cc(O)c(N(=O)=O)cc1 → 0.4 HCl + 0.4 c1cc(N(=O)=O)c([O])cc1 + 0.6 c1cc(O)c(Cl)cc1 + 0.6 NO_2	$k = 6.80 \cdot 10^{-12}$	[34]
G599	Cl + c1ccc(N(=O)=O)c(O)c1C → c1ccc(N(=O)=O)c([O])c1C + HCl	$k = 2.68 \cdot 10^{-11}$	[34], products after MCM
G600	Cl + c1cccc(O)c1C → HCl + c1cccc([O])c1C	$k = 1.10 \cdot 10^{-10}$	[34], products after MCM
G601	Cl + c1ccc(O)cc1 → HCl + c1ccc([O])cc1	$k = 1.93 \cdot 10^{-10}$	[35]
G602	Cl + c1cc(O)c(O)cc1 → HCl + c1cc(O)c([O])cc1	$k = 6.40 \cdot 10^{-10}$	[34]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G603	Cl + COC → HCl + COCO[O]	$k = 1.80 \cdot 10^{-10}$	[35]
G604	Cl + COCOO → HCl + COC=O + OH	$k = 6.10 \cdot 10^{-11}$	[36], Products after OH reaction in MCM
G605	Cl + COC=O → HCl + 0.55 C[O] + 0.45 O=COCO[O]	$k = 1.70 \cdot 10^{-11} \exp(-810/T)$	[37], products [38]
G606	Cl + CCOC=O → HCl + 0.096 CCO[O] + 0.904 CC(O[O])OC=O	$k = 5.50 \cdot 10^{-11} \exp(-556/T)$	[37], Products OH reaction MCM
G607②	Cl + C=C → ClCCO[O]	TROEF	
G608⦸	Cl + CC=C → 0.4 CC(O[O])CCl + 0.5 CC(Cl)CO[O] + 0.1 C=CCO[O]	$k = 1.43 \cdot 10^{-14} \exp(2886/T)$	[39], products after [40]
G609	CC(O[O])CCl + NO → CC([O])CCl + NO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	rate after MCM
G610	CC(Cl)CO[O] + NO → CC(Cl)C=O + NO_2 + HO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	after MCM
G611	C=CCO[O] + NO → O=CC=C + NO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	[40]
G612②	CC(O[O])CCl → 0.2 CC(O)CCl + 0.2 CC(=O)CCl + 0.6 CC([O])CCl	$k = 4.00 \cdot 10^{-14} * RO_2$	
G613	CC(Cl)C=O + OH → CC(Cl)C(=O)O[O]	$k = 4.90 \cdot 10^{-12} \exp(405/T)$	[40]
G614	CC(Cl)C=O + NO_3 → CC(Cl)C(=O)O[O] + HNO_3	$k = 3.24 \cdot 10^{-12} \exp(-1860/T)$	[40]
G615	CC(Cl)C=O → CC(Cl)O[O] + HO_2 + CO	$J = 2.879 \cdot 10^{-05} * \cos(\chi)^{1.067} \exp(-0.358/\cos(\chi))$	[40]
G616	CC(Cl)C(=O)O[O] + HO_2 → 0.15 CC(Cl)C(=O)O + 0.15 O_3 + 0.41 CC(Cl)C(=O)OO + 0.44 CC(Cl)O[O] + 0.44 OH	$k = 5.20 \cdot 10^{-13} \exp(980/T)$	[40]
G617	CC(Cl)C(=O)O[O] + NO → CC(Cl)O[O] + NO_2	$k = 7.50 \cdot 10^{-12} \exp(290/T)$	[40]
G618	CC(Cl)C(=O)O[O] + NO_2 → CC(Cl)C(=O)OON(=O)=O	TROEMCM	[40]
G619	CC(Cl)C(=O)OON(=O)=O → CC(Cl)C(=O)O[O] + NO_2	TROEMCM	after MCM
G620	CC(Cl)C(=O)O[O] + NO_3 → CC(Cl)O[O] + NO_2	$k = 4.00 \cdot 10^{-12}$	[40]
G621	CC(Cl)C(=O)O[O] → 0.3 CC(Cl)C(=O)O + 0.7 CC(Cl)O[O]	$k = 1.00 \cdot 10^{-11} * RO_2$	[40]
G622	CC(Cl)C(=O)OO + OH → CC(Cl)C(=O)O[O]	$k = 4.42 \cdot 10^{-12}$	[40]
G623	CC(Cl)C(=O)O + OH → CC(Cl)O[O]	$k = 1.20 \cdot 10^{-12}$	[40]
G624②	CC(O)CCl + OH → CC(=O)CCl + HO_2	$k = 2.60 \cdot 10^{-12} \exp(200/T)$	
G625②	CC([O])CCl → CC(=O)CCl + HO_2	$k = 1.50 \cdot 10^{-14} \exp(-230/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G626②	CC(=O)C(O)Cl + OH → CC(=O)C(=O)Cl + HO_2	k = $3.00 \cdot 10^{-12}$	
G627②	CC(Cl)(Cl)Cl + Cl → ClC(Cl)(Cl)CO[O] + HCl	k = $2.80 \cdot 10^{-12} \exp(-1790/T)$	
G628②	ClC(Cl)Cl + Cl → [O]OC(Cl)(Cl)Cl + HCl	k = $2.40 \cdot 10^{-12} \exp(-920/T)$	
G629②	[O]OC(Cl)(Cl)Cl + NO_2 → ClC(Cl)(Cl)OON(=O)=O	TROEF	
G630②	ClC(Cl)(Cl)OON(=O)=O → [O]OC(Cl)(Cl)Cl + NO_2	TROEXP	
G631②	ClCCl + Cl → [O]OC(Cl)Cl + HCl	k = $5.90 \cdot 10^{-12} \exp(-850/T)$	
G632②	O=C(Cl)Cl + OH → O=[C]Cl + HOCl	k = $5.00 \cdot 10^{-15}$	
G633②	CCl + Cl → ClCO[O] + HCl	k = $2.30 \cdot 10^{-11} \exp(-1150/T)$	
G634②	O=CCl + Cl → O=[C]Cl + HCl	k = $8.10 \cdot 10^{-12} \exp(-710/T)$	
G635②	O=[C]Cl → Cl + CO	k = [M]*$4.10 \cdot 10^{-10} \exp(2960/T)$	
G636②	Cl + CO → O=[C]Cl	k = [M]*$1.30 \cdot 10^{-33} (T/300)^{3.8}$	
G637②	Br + O_3 → BrO	k = $1.70 \cdot 10^{-11} \exp(-800/T)$	
G638②	Br + HO_2 → HBr	k = $7.70 \cdot 10^{-12} \exp(-450/T)$	
G639②	Br + H_2O_2 → HBr + HO_2	k = $1.00 \cdot 10^{-11} \exp(-3000/T)$	
G640②	Br_2 + OH → HOBr + Br	k = $2.00 \cdot 10^{-11} \exp(-240/T)$	
G641②	BrO + O_3 → 0.9 Br + 0.1 OBrO	k = $1.00 \cdot 10^{-12} \exp(-3200/T)$	
G642②	BrO + OH → Br + HO_2	k = $1.80 \cdot 10^{-11} \exp(-250/T)$	
G643②	BrO + HO_2 → HOBr	k = $4.50 \cdot 10^{-12} \exp(-500/T)$	
G644②	BrO + BrO → 1.7 Br + 0.15 Br_2	k = $1.60 \cdot 10^{-12} \exp(-210/T)$	
G645②	HBr + OH → Br	k = $6.70 \cdot 10^{-12} \exp(-155/T)$	
G646②	Br + NO_2 → $BrNO_2$	TROEF	
G647②	Br + NO_3 → BrO + NO_2	k = $1.60 \cdot 10^{-11}$	
G648②	BrO + NO → Br + NO_2	k = $8.70 \cdot 10^{-12} \exp(-260/T)$	
G649②	BrO + NO_2 → $BrNO_3$	TROEF	
G650②	$BrNO_3$ → BrO + NO_2	k = $2.79 \cdot 10^{13} \exp(-12360/T)$	
G651②	Br + $BrNO_3$ → Br_2 + NO_3	k = $4.90 \cdot 10^{-11}$	
G652②	HBr + NO_3 → Br + HNO_3	k = $1.00 \cdot 10^{-16}$	
G653②	Br + Cl_2O_2 → BrCl + ClO_2	k = $5.90 \cdot 10^{-12} \exp(-170/T)$	
G654②	Br + OClO → BrO + ClO	k = $2.70 \cdot 10^{-11} \exp(-1300/T)$	
G655②	BrO + ClO → Br + OClO	k = $1.60 \cdot 10^{-12} \exp(-430/T)$	
G656②	BrO + ClO → Br + ClO_2	k = $2.90 \cdot 10^{-12} \exp(-220/T)$	
G657②	BrO + ClO → BrCl	k = $5.80 \cdot 10^{-13} \exp(-170/T)$	
G658②	Br_2 + Cl → BrCl + Br	k = $2.30 \cdot 10^{-10} \exp(-135/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G659②	$BrCl + Br \rightarrow Br_2 + Cl$	$k = 3.32 \cdot 10^{-15}$	
G660②	$Br + Cl_2 \rightarrow BrCl + Cl$	$k = 1.10 \cdot 10^{-15}$	
G661②	$BrCl + Cl \rightarrow Br + Cl_2$	$k = 1.45 \cdot 10^{-11}$	
G662	$Br + C \rightarrow HBr + CO[O]$	$k = 5.00 \cdot 10^{-10} \exp(-8889/T)$	[41]
G663	$Br + CC \rightarrow HBr + CCO[O]$	$k = 2.35 \cdot 10^{-10} \exp(-6411/T)$	[42]
G664	$Br + CCC \rightarrow HBr + 0.44\ CCCO[O] + 0.56\ CC(O[O])C$	$k = 8.78 \cdot 10^{-11} \exp(-4330/T)$	[42], products after Cl branching
G665	$Br + CCCC \rightarrow HBr + 0.29\ CCCCO[O] + 0.71\ CCC(O[O])C$	$k = 2.86 \cdot 10^{-10} \exp(-4535/T)$	[42], products after Cl branching
G666	$Br + CC(C)C \rightarrow HBr + 0.564\ CC(C)CO[O] + 0.436\ CC(O[O])(C)C$	$k = 1.61 \cdot 10^{-10} \exp(-3464/T)$	[42], products after Cl branching
G667	$Br + CC(C)(C)C \rightarrow CC(C)(C)CO[O] + HBr$	$k = 1.14 \cdot 10^{-09} \exp(-6929/T)$	[43]
G668②	$Br + COO \rightarrow HBr + CO[O]$	$k = 2.63 \cdot 10^{-12} \exp(-1610/T)$	
G669②	$BrO + CO[O] \rightarrow 0.25\ Br + 0.25\ C{=}O + 0.25\ HO_2 + 0.75\ HOBr + 0.75\ O{=}CO$	$k = 4.10 \cdot 10^{-13} \exp(-800/T)$	
G670②	$Br + C\#C \rightarrow 0.17\ O{=}CBr + 0.09\ Br + 0.74\ HBr + 0.09\ O{=}CC{=}O + 1.65\ CO + 0.91\ HO_2$	$k = 6.35 \cdot 10^{-15} \exp(-440/T)$	
G671	$Br + COC \rightarrow HBr + COCO[O]$	$k = 1.71 \cdot 10^{-15}$	[44]
G672②	$Br + C{=}O \rightarrow HBr + CO + HO_2$	$k = 1.70 \cdot 10^{-11} \exp(-800/T)$	
G673②	$BrO + C{=}O \rightarrow HOBr + CO + HO_2$	$k = 1.50 \cdot 10^{-14}$	
G674②	$Br + CC{=}O \rightarrow HBr + CCC(=O)O[O]$	$k = 1.80 \cdot 10^{-11} \exp(-460/T)$	
G675	$Br + CCC{=}O \rightarrow HBr + CC(=O)O[O]$	$k = 5.75 \cdot 10^{-11} \exp(-610/T)$	[45]
G676	$Br + CCCC{=}O \rightarrow HBr + CCCC(=O)O[O]$	$k = 5.75 \cdot 10^{-11} \exp(-540/T)$	[45]
G677	$Br + CC(C)C{=}O \rightarrow HBr + CC(C)C(=O)O[O]$	$k = 6.30 \cdot 10^{-12}$	[46]
G678	$Br + CC(C)(C)C{=}O \rightarrow HBr + CC(C)(C)C(=O)O[O]$	$k = 8.50 \cdot 10^{-12}$	[46]
G679	$Br + CC(=O)C \rightarrow HBr + CC(=O)CO[O]$	$k = 4.53 \cdot 10^{-20}$	[47]
G680	$Br + O{=}CC{=}O \rightarrow HBr + O{=}CC(=O)O[O]$	$k = 1.40 \cdot 10^{-14}$	[48]
G681	$Br + O{=}CC{=}C \rightarrow 0.2\ HBr + 0.2\ C{=}CC(=O)O[O] + 0.8\ BrCC(O[O])C{=}O$	$k = 3.21 \cdot 10^{-12}$	[49]
G682	$BrCC(O[O])C{=}O + NO \rightarrow BrCC{=}O + HO_2 + CO + NO_2$	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	Rate constant MCM, products [10]
G683	$BrCC(O[O])C{=}O + NO_3 \rightarrow$	$k = 2.30 \cdot 10^{-12}$	Rate constant MCM, products [10]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	BrCC=O + HO_2 + CO + NO_2		
G684	BrCC(O[O])C=O → BrCC=O + HO_2 + CO	k = $8.80 \cdot 10^{-13} * RO_2$	Rate constant MCM, products [10]
G685⦸	Br + c1ccccc1C → HBr + c1ccccc1CO[O]	k = $3.70 \cdot 10^{-12} \exp(-1630/T)$	[50]
G686	Br + Cc1ccccc1C → HBr + Cc1ccccc1CO[O]	k = $8.90 \cdot 10^{-14}$	[51]
G687	Br + c1c(C)cccc1C → Cc1cccc(c1)CO[O] + HBr	k = $6.60 \cdot 10^{-14}$	[51]
G688	Br + c1cc(C)ccc1C → Cc1ccc(CO[O])cc1 + HBr	k = $9.00 \cdot 10^{-14}$	[51]
G689	Br + c1c(C)cc(C)cc1C → c1c(C)cc(CO[O])cc1C + HBr	k = $4.80 \cdot 10^{-13}$	[51]
G690	Br + OC → HBr + C=O + HO_2	k = $5.00 \cdot 10^{-16}$	[51]
G691	Br + CCO → 0.95 CC=O + 0.95 HO_2 + 0.05 OCCO[O] + HBr	k = $9.80 \cdot 10^{-15}$	[51]
G692	Br + CCCO → 0.69 CCC=O + 0.69 HO_2 + 0.06 OCCCO[O] + 0.25 CC(O[O])CO + HBr	k = $8.30 \cdot 10^{-15}$	[51]
G693	Br + CC(O)C → CC(=O)C + HBr	k = $4.60 \cdot 10^{-14}$	[51]
G694	Br + CC(O)(C)C → HBr + 0.888 CC(O)(C)CO[O] + 0.112 CC([O])(C)C	k = $5.00 \cdot 10^{-16}$	[51]
G695②	Br + C=C → BrCCO[O]	k = $2.25 \cdot 10^{-13} \exp(-277/T)$	
G696②	BrCCO[O] → 0.2 OCCBr + 0.2 BrCC=O + 0.6 BrCC[O]	k = $2.00 \cdot 10^{-12} * RO_2$	
G697②	BrCCO[O] + NO → BrCC[O] + NO_2	k = $9.70 \cdot 10^{-12}$	
G698②	OCCBr + OH → BrCC=O + HO_2	k = $4.60 \cdot 10^{-12}$	
G699②	BrCC[O] → BrCC=O + HO_2	k = $6.00 \cdot 10^{-14} \exp(-550/T)$	
G700②	Br + CC=C → CC(O[O])CBr	k = $3.60 \cdot 10^{-12}$	
G701②	CC(O[O])CBr → 0.2 CC(O)CBr + 0.2 CC(=O)CBr + 0.6 CC([O])CBr	k = $4.00 \cdot 10^{-14} * RO_2$	
G702②	CC(O[O])CBr + NO → CC([O])CBr + NO_2	k = $2.70 \cdot 10^{-12} \exp(360/T)$	
G703②	CC(O)CBr + OH → CC(=O)CBr + HO_2	k = $2.60 \cdot 10^{-12} \exp(200/T)$	
G704②	CC([O])CBr → CC(=O)CBr + HO_2	k = $1.50 \cdot 10^{-14} \exp(-230/T)$	
G705②	CC(=O)CBr + OH → CC(=O)C(Br)O[O]	k = $8.80 \cdot 10^{-12} \exp(-1320/T)$	
G706②	CC(=O)C(Br)O[O] → 0.2 CC(=O)C(O)Br + 0.2 CC(=O)C(=O)Br + 0.6 CC(=O)O[O] + 0.6 O=CBr	k = $2.00 \cdot 10^{-12} * RO_2$	
G707②	CC(=O)C(Br)O[O] + NO →	k = $8.00 \cdot 10^{-12}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	CC(=O)O[O] + O=CBr + NO_2		
G708②	CC(=O)C(O)Br + OH → CC(=O)C(=O)Br + HO_2	k = $3.00 \cdot 10^{-12}$	
G709②	BrC(Br)Br + OH → BrC(Br)(Br)O[O]	k = $1.35 \cdot 10^{-12} \exp(-600/T)$	
G710②	BrC(Br)Br + Cl → BrC(Br)(Br)O[O] + HCl	k = $4.85 \cdot 10^{-12} \exp(-850/T)$	
G711②	BrC(Br)(Br)O[O] + HO_2 → O=C(Br)Br + HOBr	k = $4.70 \cdot 10^{-13} \exp(710/T)$	
G712②	BrC(Br)(Br)O[O] → 0.3 OC(Br)(Br)Br + 0.7 BrC(Br)(Br)[O]	k = $6.60 \cdot 10^{-12} * RO_2$	
G713②	BrC(Br)(Br)O[O] + NO → O=C(Br)Br + Br + NO_2	k = $7.30 \cdot 10^{-12} \exp(270/T)$	
G714②	BrC(Br)(Br)O[O] + NO_2 → BrC(Br)(Br)OON(=O)=O	TROEF	
G715②	BrC(Br)(Br)OON(=O)=O → BrC(Br)(Br)O[O] + NO_2	TROEXP	
G716②	OC(Br)(Br)Br + OH → BrC(Br)(Br)[O]	k = $3.60 \cdot 10^{-14}$	
G717②	BrC(Br)(Br)[O] → O=C(Br)Br + Br	k = $4.00 \cdot 10^{13} \exp(-4600/T)$	
G718②	BrCBr + OH → BrC(Br)O[O]	k = $1.50 \cdot 10^{-12} \exp(-775/T)$	
G719②	BrCBr + Cl → BrC(Br)O[O] + HCl	k = $6.30 \cdot 10^{-12} \exp(-800/T)$	
G720②	BrC(Br)O[O] + HO_2 → 0.3 O=CBr + 0.3 HOBr + 0.7 O=C(Br)Br	k = $5.60 \cdot 10^{-13} \exp(700/T)$	
G721②	BrC(Br)O[O] → 0.2 O=C(Br)Br + 0.2 OC(Br)Br + 0.6 O=CBr + 0.6 Br + 0.6 HO_2	k = $2.00 \cdot 10^{-12} * RO_2$	
G722②	BrC(Br)O[O] + NO → O=CBr + Br + NO_2	k = $1.70 \cdot 10^{-11}$	
G723②	OC(Br)Br + OH → O=C(Br)Br + HO_2	k = $9.34 \cdot 10^{-13}$	
G724②	O=C(Br)Br + OH → O=[C]Br + HOBr	k = $5.00 \cdot 10^{-15}$	
G725②	CBr + OH → BrCO[O] + H_2O	k = $7.40 \cdot 10^{-13} \exp(-875/T)$	implemented from MCM
G726②	CBr + Cl → BrCO[O] + HCl	k = $1.40 \cdot 10^{-11} \exp(-1030/T)$	
G727②	BrCO[O] + HO_2 → BrCOO	k = $4.28 \cdot 10^{-13} \exp(820/T)$	
G728②	BrCO[O] + NO → BrC[O] + NO_2	k = $4.05 \cdot 10^{-12} \exp(360/T)$	
G729☒	BrCO[O] + NO_3 → BrC[O] + NO_2	k = $2.30 \cdot 10^{-12}$	
G730②	BrCO[O] → 0.6 BrC[O] + 0.2 OCBr + 0.2 O=CBr	k = $2.00 \cdot 10^{-12} * RO_2$	
G731②	BrCOO + OH → BrCO[O] + H_2O	k = $1.90 \cdot 10^{-12} \exp(190/T)$	
G732②	BrCOO + OH → O=CBr + OH + H_2O	k = $5.79 \cdot 10^{-12}$	
G733②	BrCOO → BrC[O] + OH	J = $7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	implemented from MCM
G734②	BrC[O] + O_2 → O=CBr + HO_2	k = $2.50 \cdot 10^{-14} \exp(-300/T)$	implemented from MCM
G735②	OCBr + OH → O=CBr + HO_2 + H_2O	k = $1.06 \cdot 10^{-12}$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G736☒	$O=CBr + NO_3 \rightarrow CO + Br + HNO_3$	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	
G737②	$O=CBr + OH \rightarrow CO + Br + H_2O$	$k = 1.16 \cdot 10^{-12}$	
G738②	$O=CBr + Cl \rightarrow O=[C]Br + HCl$	$k = 8.10 \cdot 10^{-12} \exp(-710/T)$	
G739②	$O=CBr \rightarrow HO_2 + CO + Br$	$J = 4.642 \cdot 10^{-05} * \cos(\chi)^{0.762} \exp(-0.353/\cos(\chi))$	implemented from MCM
G740②	$O=[C]Br \rightarrow Br + CO$	$k = [M] * 4.10 \cdot 10^{-10} \exp(2960/T)$	
G741②	$Br + CO \rightarrow O=[C]Br$	$k = [M] * 1.30 \cdot 10^{-33} (T/300)^{3.8}$	
G742☒	$BrCCBr + OH \rightarrow BrCC(Br)O[O] + H_2O$	$k = 1.03 \cdot 10^{-17} * T^2 \exp(-422/T)$	
G743☒	$BrCC(Br)O[O] + HO_2 \rightarrow BrCC(Br)OO$	$k = 3.30 \cdot 10^{-13} \exp(820/T)$	
G744☒	$BrCC(Br)O[O] + NO \rightarrow BrCC(Br)[O] + NO_2$	$k = 4.05 \cdot 10^{-12} \exp(360/T)$	
G745☒	$BrCC(Br)O[O] + NO_3 \rightarrow BrCC(Br)[O] + NO_2$	$k = 2.30 \cdot 10^{-12}$	
G746☒	$BrCC(Br)O[O] \rightarrow$ 0.2 $BrCC{=}O$ + 0.6 $BrCC(Br)[O]$ + 0.2 $BrCC(O)Br$	$k = 8.80 \cdot 10^{-13} * RO_2$	
G747☒	$BrCC(Br)OO + OH \rightarrow BrCC(Br)O[O] + H_2O$	$k = 9.52 \cdot 10^{-12}$	
G748☒	$BrCC(Br)OO \rightarrow BrCC(Br)[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	
G749☒	$BrCC(Br)[O] \rightarrow BrCC{=}O + Br$	$k = 1.00 \cdot 10^{+06}$	
G750☒	$BrCC{=}O + NO_3 \rightarrow BrCC(=O)O[O] + HNO_3$	$k = 1.40 \cdot 10^{-12} \exp(-1860/T)$	
G751②	$BrCC{=}O + OH \rightarrow BrCC(=O)O[O] + H_2O$	$k = 2.05 \cdot 10^{-12}$	implemented from MCM
G752☒	$BrCC{=}O \rightarrow BrCO[O] + HO_2 + CO$	$J = 4.642 \cdot 10^{-05} * \cos(\chi)^{0.762} \exp(-0.353/\cos(\chi))$	
G753☒	$BrCC(O)Br + OH \rightarrow BrCC(Br)[O] + H_2O$	$k = 2.80 \cdot 10^{-12}$	
G754②	$BrCC(=O)O[O] + HO_2 \rightarrow$ 0.15 $BrCC(=O)O$ + 0.15 O_3 + 0.41 $BrCC(=O)OO$ + 0.44 $BrCO[O]$ + 0.44 OH	$k = 5.20 \cdot 10^{-13} \exp(980/T)$	implemented from MCM
G755②	$BrCC(=O)O[O] + NO \rightarrow BrCO[O] + NO_2$	$k = 7.50 \cdot 10^{-12} \exp(290/T)$	implemented from MCM
G756②	$BrCC(=O)O[O] + NO_2 \rightarrow BrCC(=O)OON(=O)=O$	TROEMCM	implemented from MCM
G757☒	$BrCC(=O)O[O] + NO_3 \rightarrow BrCO[O] + NO_2$	$k = 4.00 \cdot 10^{-12}$	
G758②	$BrCC(=O)O[O] \rightarrow$ 0.3 $BrCC(=O)O$ + 0.7 $BrCO[O]$	$k = 1.00 \cdot 10^{-11} * RO_2$	implemented from MCM
G759②	$BrCC(=O)O + OH \rightarrow BrCO[O] + H_2O$	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G760②	$BrCC(=O)OO + OH \rightarrow BrCC(=O)O[O] + H_2O$	$k = 3.79 \cdot 10^{-12}$	implemented from MCM
G761②	$BrCC(=O)OO \rightarrow BrCO[O] + OH$	$J = 7.649 \cdot 10^{-06} * \cos(\chi)^{0.682} \exp(-0.279/\cos(\chi))$	implemented from MCM
G762②	$BrCC(=O)OON(=O)=O + OH \rightarrow$ $O=CBr + CO + NO_2$	$k = 5.56 \cdot 10^{-13}$	implemented from MCM
G763②	$BrCC(=O)OON(=O)=O \rightarrow$	TROEMCM	implemented from MCM

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	BrCC(=O)O[O] + NO_2		
G764②	I + I → I_2	k = $2.99 \cdot 10^{-11}$	
G765②	I + O_3 → IO	k = $2.10 \cdot 10^{-11} \exp(-830/T)$	
G766②	I_2 + OH → I + HOI	k = $2.10 \cdot 10^{-10}$	
G767②	I + HO_2 → HI	k = $1.50 \cdot 10^{-11} \exp(-1090/T)$	
G768②	IO + HO_2 → HOI	k = $1.40 \cdot 10^{-11} \exp(540/T)$	
G769⦸	IO + IO → 0.38 OIO + 0.46 I_2O_2 + 0.6 I + 0.05 I_2	k = $5.40 \cdot 10^{-11} \exp(180/T)$	revised after IUPAC
G770⦸	OIO + OH → HIO_3	k = $2.20 \cdot 10^{-10} \exp(243/T)$	revised after [52]
G771	IO + O_3 → 0.83 I + 0.17 OIO	k = $1.20 \cdot 10^{-15}$	[53], branching ratios IUPAC
G772	IO + OIO → I_2O_3	k = $1.00 \cdot 10^{-10}$	[54]
G773	I_2O_3 → IO + OIO	k = $2.78 \cdot 10^{-11}$	[55] (upper limit)
G774	OIO + OIO → I_2O_4	k = $1.00 \cdot 10^{-10}$	[56]
G775	I_2O_4 → OIO + OIO	k = $1.67 \cdot 10^{+00}$	[55] (upper limit)
G776	I_2 + O_3 → IO + I	k = $4.02 \cdot 10^{-15} \exp(-2050/T)$	[57], products [58]
G777⦸	I_2O_2 → 0.995 OIO + 0.995 I + 0.01 IO	k = $1.00 \cdot 10^{+01}$	revised after [55]
G778②	HI + OH → I + H_2O	k = $1.60 \cdot 10^{-11} \exp(440/T)$	
G779②	I + NO → INO	TROE	
G780②	I + NO_2 → INO_2	TROEF	
G781②	I + NO_3 → IO + NO_2	k = $4.50 \cdot 10^{-10}$	
G782②	I_2 + NO_3 → I + INO_3	k = $1.50 \cdot 10^{-12}$	
G783②	IO + NO → I + NO_2	k = $7.15 \cdot 10^{-12} \exp(300/T)$	
G784②	IO + NO_2 → INO_3	TROEF	
G785②	OIO + NO → IO + NO_2	k = $1.10 \cdot 10^{-12} \exp(542/T)$	
G786②	HI + NO_3 → I + HNO_3	k = $1.30 \cdot 10^{-12} \exp(-1830/T)$	
G787②	INO + INO → I_2 + 2.0 NO	k = $8.40 \cdot 10^{-11} \exp(-2620/T)$	
G788②	INO_2 + INO_2 → I_2 + 2.0 NO_2	k = $4.70 \cdot 10^{-13} \exp(-1670/T)$	
G789②	INO_2 → I + NO_2	k = [M]*$9.60 \cdot 10^{-20}$	
G790②	INO_3 → IO + NO_2	k = [M]*$4.40 \cdot 10^{-05} \exp(12060/T)$	
G791②	IO + CO[O] → I + HO_2 + C=O	k = $2.00 \cdot 10^{-12}$	
G792②	I_2 + Cl → I + ICl	k = $2.10 \cdot 10^{-10}$	
G793②	I_2 + Br → I + IBr	k = $1.20 \cdot 10^{-10}$	
G794②	I + BrO → IO + Br	k = $1.20 \cdot 10^{-11}$	
G795②	IO + ClO → 0.8 I + 0.55 OClO + 0.25 Cl + 0.2 ICl	k = $4.70 \cdot 10^{-12} \exp(280/T)$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
G796	IO + Cl → ClO + I	$k = 4.40 \cdot 10^{-11}$	[59]
G797②	IO + BrO → 0.8 OIO + Br + 0.2 I	$k = 1.50 \cdot 10^{-11} \exp(510/T)$	
G798	IO + Br → BrO + I	$k = 2.50 \cdot 10^{-11}$	[60]
G799	OIO + Br → BrO + IO	$k = 3.00 \cdot 10^{-12}$	[60]
G800⦸	CC(I)C + OH → CC(O[O])(I)C + H_2O	$k = 7.64 \cdot 10^{-12} \exp(-530/T)$	revised after IUPAC
G801②	CC(O[O])(I)C → CC([O])(I)C	$k = 2.40 \cdot 10^{-14} * RO_2$	
G802②	CC(O[O])(I)C + NO → CC([O])(I)C + NO_2	$k = 2.70 \cdot 10^{-12} \exp(360/T)$	
G803②	CC([O])(I)C → CC(=O)C + I	$k = 1.00 \cdot 10^{+01}$	
G804⦸	ICC + OH → 0.13 CC(O[O])I + 0.87 ICCO[O] + H_2O	$k = 5.65 \cdot 10^{-11} \exp(-841/T)$	revised after IUPAC
G805②	ICCO[O] → 0.2 ICCO + 0.2 ICC=O + 0.6 ICC[O]	$k = 2.00 \cdot 10^{-12} * RO_2$	
G806②	ICCO[O] + NO → ICC[O] + NO_2	$k = 9.70 \cdot 10^{-12}$	
G807②	ICCO + OH → ICC=O + HO_2 + H_2O	$k = 4.60 \cdot 10^{-12}$	
G808②	ICC[O] → ICC=O + HO_2	$k = 6.00 \cdot 10^{-14} \exp(-550/T)$	
G809②	ICC=O + OH → ICC(=O)O[O] + H_2O	$k = 3.10 \cdot 10^{-12}$	
G810②	ICC(=O)O[O] + HO_2 → 0.29 ICC(=O)O + 0.29 O_3 + 0.71 ICC(=O)OO	$k = 4.30 \cdot 10^{-13} \exp(1040/T)$	
G811②	ICC(=O)O[O] → 0.7 [O]OCI + 0.7 CO_2 + 0.3 ICC(=O)O	$k = 1.00 \cdot 10^{-11} * RO_2$	
G812②	ICC(=O)O[O] + NO → [O]OCI + CO_2 + NO_2	$k = 8.10 \cdot 10^{-12} \exp(270/T)$	
G813②	ICC(=O)O[O] + NO_2 → ICC(=O)OON(=O)=O	TROEF	
G814②	ICC(=O)OON(=O)=O → ICC(=O)O[O] + NO_2	TROEXP	
G815②	ICC(=O)OON(=O)=O + OH → O=C(OON(=O)(=O))C(O[O])I + H_2O	$k = 6.26 \cdot 10^{-13}$	
G816②	O=C(OON(=O)(=O))C(O[O])I + NO → O=CI + CO + 2.0 NO_2	$k = 4.064 \cdot 10^{-12} \exp(360/T)$	
G817②	ICC(=O)OO + OH → ICC(=O)O[O] + H_2O	$k = 4.29 \cdot 10^{-12}$	
G818②	ICC(=O)O + OH → [O]OCI + CO_2 + H_2O	$k = 1.90 \cdot 10^{-12} \exp(190/T)$	
G819②	CC(O[O])I →	$k = 8.80 \cdot 10^{-13} * RO_2$	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1, ☒ implemented from MCMv3.2

Nr.	Reaction	Rate constant	Reference
	0.2 CC(O)I + 0.2 CC(=O)I + 0.6 CC=O + 0.6 I + 0.6 HO_2		
G820②	CC(O[O])I + NO → CC=O + I + NO_2	k = $5.59 \cdot 10^{-12} \exp(360/T)$	
G821②	CC(O)I + OH → CC(=O)I + HO_2 + H_2O	k = $2.77 \cdot 10^{-12}$	
G822②	CC(=O)I + OH → O=C(I)CO[O] + H_2O	k = $3.88 \cdot 10^{-14}$	
G823②	O=C(I)CO[O] → I + CO + C=O + HO_2	k = $2.00 \cdot 10^{-12} * RO_2$	
G824②	O=C(I)CO[O] + NO → I + CO + C=O + NO_2	k = $4.064 \cdot 10^{-12} \exp(360/T)$	
G825⦸	ICI + OH → IC(I)O[O] + H_2O	k = $4.20 \cdot 10^{-11} \exp(-670/T)$	61
G826	ICI + NO_3 → IC(I)O[O] + HNO_3	k = $4.00 \cdot 10^{-13}$	62
G827⦸	ICI + Cl → 0.55 IC(I)O[O] + 0.55 HCl + 0.45 [O]OCI + 0.45 ICl	k = $4.70 \cdot 10^{-11} \exp(-241/T)$	63
G828②	IC(I)O[O] + HO_2 → 0.3 O=CI + 0.3 HOI + 0.7 O=C(I)I	k = $5.60 \cdot 10^{-13} \exp(700/T)$	
G829②	IC(I)O[O] → 0.2 O=C(I)I + 0.2 IC(I)O + 0.6 O=CI + 0.6 I + 0.6 HO_2	k = $2.00 \cdot 10^{-12} * RO_2$	
G830②	IC(I)O[O] + NO → O=CI + I + NO_2	k = $1.70 \cdot 10^{-11}$	
G831②	IC(I)O + OH → O=C(I)I + HO_2 + H_2O	k = $9.34 \cdot 10^{-13}$	
G832②	O=C(I)I + OH → O=[C]I + HOI + H_2O	k = $5.00 \cdot 10^{-15}$	
G833②	CI + OH → [O]OCI + H_2O	k = $4.30 \cdot 10^{-12} \exp(-1120/T)$	
G834②	CI + Cl → [O]OCI + HCl	k = $2.90 \cdot 10^{-11} \exp(-1000/T)$	
G835②	CI + NO_3 → [O]OCI + HNO_3	k = $1.00 \cdot 10^{-17}$	
G836②	[O]OCI + HO_2 → 0.85 OOCI + 0.15 O=CI	k = $6.70 \cdot 10^{-12}$	
G837②	[O]OCI → 0.2 OCI + 0.2 O=CI + 0.6 [O]CI	k = $2.00 \cdot 10^{-12} * RO_2$	
G838②	[O]OCI + NO → [O]CI + NO_2	k = $1.10 \cdot 10^{-11}$	
G839②	OOCI + OH → [O]OCI + H_2O	k = $1.90 \cdot 10^{-12} \exp(190/T)$	
G840②	OOCI + OH → O=CI + OH + H_2O	k = $5.79 \cdot 10^{-12}$	
G841②	OCI + OH → O=CI + HO_2 + H_2O	k = $1.06 \cdot 10^{-12}$	
G842②	[O]CI → O=CI + HO_2	k = $6.00 \cdot 10^{-14} \exp(-550/T)$	
G843②	O=CI + OH → I + CO + H_2O	k = $1.16 \cdot 10^{-12}$	
G844②	O=CI + Cl → O=[C]I + HCl	k = $8.10 \cdot 10^{-12} \exp(-710/T)$	
G845②	O=[C]I → I + CO	k = [M]*$4.10 \cdot 10^{-10} \exp(2960/T)$	
G846②	I + CO → O=[C]I	k = [M]*$1.30 \cdot 10^{-33} (T/300)^{3.8}$	

Parameters for pressure dependent reactions.

	Reaction	TYPE	k_0	$k\infty$	F_C
G307	$ClC(Cl)(Cl)C(=O)O[O] + NO_2 \rightarrow O=N(=O)OOC(=O)C(Cl)(Cl)Cl$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G313	$ClCC(=O)O[O] + NO_2 \rightarrow ClCC(=O)OON(=O)=O$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G318	$OC(Cl)(Cl)C(=O)O[O] + NO_2 \rightarrow O=N(=O)OOC(=O)C(O)(Cl)Cl$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G323	$ClCC(Cl)C(=O)O[O] + NO_2 \rightarrow ClCC(Cl)C(=O)OON(=O)=O$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G334	$ClC(Cl)C(=O)O[O] + NO_2 \rightarrow O=N(=O)OOC(=O)C(Cl)Cl$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G353	$OC(Cl)C(=O)O[O] + NO_2 \rightarrow O=N(=O)OOC(=O)C(O)Cl$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G358	$O=N(=O)OOC(=O)C(Cl)(Cl)Cl \rightarrow ClC(Cl)(Cl)C(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G363	$ClCC(=O)OON(=O)=O \rightarrow ClCC(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G367	$O=N(=O)OOC(=O)C(O)(Cl)Cl \rightarrow OC(Cl)(Cl)C(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G372	$ClCC(Cl)C(=O)OON(=O)=O \rightarrow ClCC(Cl)C(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G384	$O=N(=O)OOC(=O)C(Cl)Cl \rightarrow ClC(Cl)C(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G400	$O=N(=O)OOC(=O)C(O)Cl \rightarrow OC(Cl)C(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G468	$ClO + ClO \rightarrow Cl_2O_2$	TROE	$1.60\cdot10^{-32}*(T/298)^{-4.5}$	$2.00\cdot10^{-12}*(T/298)-2.4$	
G469	$Cl + O_2 \rightarrow ClO_2$	TROE	$2.20\cdot10^{-33}*(T/298)^{-3.1}$	$1.80\cdot10^{-10}$	
G472	$Cl_2O_2 \rightarrow ClO + ClO$	TROEXP	$3.70\cdot10^{-07}\exp(-7690/T)$	$7.90\cdot10^{+15}\exp(-8820/T)$	0.45
G477	$OClO + ClO \rightarrow Cl_2O_3$	TROE	$6.20\cdot10^{-32}*(T/298)^{-4.7}$	$2.40\cdot10^{-11}$	
G478	$Cl_2O_3 \rightarrow OClO + ClO$	TROEXP	1.40·10-10exp(-3810/T)	$2.50\cdot10^{+12}\exp(-4940/T)$	
G488	$Cl + NO_2 \rightarrow ClNO_2$	TROE	$1.80\cdot10^{-31}*(T/298)^{-2.0}$	$1.00\cdot10^{-10}*(T/298)^{-1.0}$	
G490	$ClO + NO_2 \rightarrow ClNO_3$	TROEF	$1.60\cdot10^{-31}*(T/298)^{-3.4}$	$7.00\cdot10^{-11}$	0.4
G570	$Cl + C\#C \rightarrow 0.26\ O=CCl + 0.21\ Cl + 0.53\ HCl + 0.21\ O=CC=O + 1.32\ CO + 0.79\ HO_2$	TROE	$6.10\cdot10^{-30}*(T/298)^{-3.0}$	$2.00\cdot10^{-10}$	
G607	$Cl + C=C \rightarrow ClCCO[O]$	TROEF	$1.85\cdot10^{-29}*(T/298)^{-3.3}$	$6.00\cdot10^{-10}$	0.4
G618	$CC(Cl)C(=O)O[O] + NO_2 \rightarrow CC(Cl)C(=O)OON(=O)=O$	TROEMCM	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
G619	$CC(Cl)C(=O)OON(=O)=O \rightarrow CC(Cl)C(=O)O[O] + NO_2$	TROEMCM	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
G629	$[O]OC(Cl)(Cl)Cl + NO_2 \rightarrow ClC(Cl)(Cl)OON(=O)=O$	TROEF	$9.20\cdot10^{-29}*(T/298)^{-6.0}$	$1.50\cdot10^{-12}*(T/298)^{-0.7}$	0.32
G630	$ClC(Cl)(Cl)OON(=O)=O \rightarrow [O]OC(Cl)(Cl)Cl + NO_2$	TROEXP	$4.30\cdot10^{-03}\exp(-10235/T)$	$4.80\cdot10^{+16}\exp(-13830/T)$	0.32
G646	$Br + NO_2 \rightarrow BrNO_2$	TROEF	$4.20\cdot10^{-31}*(T/298)^{-2.4}$	$2.70\cdot10^{-11}$	0.55
G649	$BrO + NO_2 \rightarrow BrNO_3$	TROEF	$4.70\cdot10^{-31}*(T/298)^{-3.1}$	$1.80\cdot10^{-11}$	0.4
G714	$BrC(Br)(Br)O[O] + NO_2 \rightarrow BrC(Br)(Br)OON(=O)=O$	TROEF	$9.20\cdot10^{-29}*(T/298)^{-6.0}$	$1.50\cdot10^{-12}*(T/298)^{-0.7}$	0.32
G715	$BrC(Br)(Br)OON(=O)=O \rightarrow BrC(Br)(Br)O[O] + NO_2$	TROEXP	$4.30\cdot10^{-03}\exp(-10235/T)$	$4.80\cdot10^{+16}\exp(-11820/T)$	0.32

	Reaction	TYPE	k_0	$k\infty$	F_C
G756	BrCC(=O)O[O] + NO_2 → BrCC(=O)OON(=O)=O	TROEMCM	$2.70 \cdot 10^{-28} * (T/298)^{7.1}$	$1.20 \cdot 10^{-11} * (T/298)^{0.9}$	0.3
G763	BrCC(=O)OON(=O)=O → BrCC(=O)O[O] + NO_2	TROEMCM	$4.90 \cdot 10^{-03} \exp(-12100/T)$	$5.40 \cdot 10^{+16} \exp(-13830/T)$	0.3
G779	I + NO → INO	TROE	$1.80 \cdot 10^{-32} * (T/298)^{-1.0}$	$1.70 \cdot 10^{-11}$	
G780	I + NO_2 → INO_2	TROEF	$3.00 \cdot 10^{-31} * (T/298)^{-1.0}$	$6.60 \cdot 10^{-11}$	
G784	IO + NO_2 → INO_3	TROEF	$7.70 \cdot 10^{-31} (T/300)^{-5.0}$	$1.60 \cdot 10^{-11}$	
G813	ICC(=O)O[O] + NO_2 → ICC(=O)OON(=O)=O	TROEF	$2.70 \cdot 10^{-28} * (T/298)^{7.1}$	$1.20 \cdot 10^{-11} * (T/298)^{0.9}$	0.3
G814	ICC(=O)OON(=O)=O → ICC(=O)O[O] + NO_2	TROEXP	$4.90 \cdot 10^{-03} \exp(-12100/T)$	$5.40 \cdot 10^{+16} \exp(-13830/T)$	0.3

Uptake processes implemented within the CAPRAM-HM3.0.

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Species	$K_{H\,298}$, [M atm^{-1}]	-ΔH/R, [K]	Ref.	α	Ref.	$D_{g\,298}$ [10^5 m^2 s^{-1}]	Ref.
H1②	Cl_2	$9.15 \cdot 10^{-2}$	2490	[64]	0.08	[64]	1.28	[64]
H2②	Cl	$2.00 \cdot 10^{-1}$		[64]	0.05	[64]	1.82	[64]
H3⦸	ClO	$5.50 \cdot 10^{0}$		[65]	0.064	[64]	1.55	[64]
H4②	ClO_2	$1.00 \cdot 10^{0}$	-3300	[64]	0.05	[64]	1.39	[64]
H5②	HCl	$1.10 \cdot 10^{0}$	2020	[64]	0.1026	[64]	1.89	[64]
H6②	HOCl	$6.60 \cdot 10^{2}$	5862	[64]	0.5	[64]	1.51	[64]
H7②	ClNO	$5.00 \cdot 10^{-2}$		[64]	0.01	[64]	1.39	[64]
H8②	$ClNO_2$	$2.40 \cdot 10^{-2}$		[64]	0.01	[64]	1.27	[64]
H9②	$ClNO_3$	$2.10 \cdot 10^{5}$	8700	[64]	0.1	[64]	1.18	[64]
H10②	$ClCH_2CO(O_2)$	$6.69 \cdot 10^{2}$	5893	[64]	0.019	[64]	0.94	[64]
H11⦸	$ClCH_2COOH$	$1.11 \cdot 10^{5}$	9700	[66]	0.1	[64]	0.97	[64]
H12②	$CH_3COCOCl$	$1.40 \cdot 10^{0}$	7541	[64]	0.03	[64]	0.88	[64]
H13⦸	$COCl_2$	$5.98 \cdot 10^{-2}$	3800	[67]	0.02	[64]	1.02	[64]
H14②	CHOCl	$3.00 \cdot 10^{3}$	7216	[64]	0.02	[64]	1.23	[64]
H15	$ClCH_2CHO$	$4.15 \cdot 10^{1}$		[66]	0.03	as CH_3CHO	1.19	[68]
H16	Cl_2CHCHO	$1.22 \cdot 10^{2}$		[66]	0.03	as CH_3CHO	1.16	[68]
H17	CH_3COCl	$4.15 \cdot 10^{1}$		estimated as $ClCH_2CHO$	0.03	as CH_3CHO	1.19	[68]
H18	$ClCH_2COCl$	$4.36 \cdot 10^{0}$		[66]	0.03	as CH_3CHO	1.16	[68]
H19	$ClCH_2CH_2OH$	$9.63 \cdot 10^{3}$		[66]	0.0176	as CH_3CH_2OH	1.14	[68]
H20	$CH_3CHOHCH_2Cl$	$5.88 \cdot 10^{2}$		[66]	0.013	as $CH_3CHOHCH_3$	0.98	[68]
H21	Cl_3CCHO	$3.45 \cdot 10^{5}$	3500	[66]	0.03	as CH_3CHO	1.15	[68]
H22	CH_3COCH_2Cl	$5.88 \cdot 10^{1}$	5400	[66]	0.0054	as CH_3COCH_3	1.00	[68]
H23	$Cl_2CHCOOH$	$1.22 \cdot 10^{5}$	8000	[66]	0.1	as $ClCH_2COOH$	1.09	[68]
H24	o-C_6H_5ClO	$1.52 \cdot 10^{2}$		[66]	0.1	estimated	0.77	[68]
H25	p-C_6H_5ClO	$1.42 \cdot 10^{5}$	11000	[66]	0.1	estimated	0.77	[68]
H26②	Br_2	$7.60 \cdot 10^{-1}$	4100	[64]	0.08	[64]	1.00	[64]
H27②	Br	$1.20 \cdot 10^{0}$		[64]	0.05	[64]	1.29	[64]
H28⦸	BrO	$5.50 \cdot 10^{0}$		estimated as ClO	0.06	[64]	1.19	[64]
H29②	HBr	$1.30 \cdot 10^{0}$	10239	[64]	0.0481	[64]	1.26	[64]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Species	$K_{H\,298}$, [M atm^{-1}]	-ΔH/R, [K]	Ref.	α	Ref.	$D_{g\,298}$ [10^5 m^2 s^{-1}]	Ref.
H30②	HOBr	$9.30 \cdot 10^{1}$	5862	[64]	0.5	[64]	1.16	[64]
H31②	$BrNO_2$	$3.00 \cdot 10^{-1}$		[64]	0.01	[64]	1.06	[64]
H32②	$BrNO_3$	$2.10 \cdot 10^{5}$	8700	[64]	0.8	[64]	1.01	[64]
H33②	BrCl	$9.40 \cdot 10^{-1}$	-5600	[64]	0.33	[64]	1.05	[64]
H34②	$BrCH_2CO(O_2)$	$6.69 \cdot 10^{2}$	5893	[64]	0.019	[64]	0.84	[64]
H35⦸	$BrCH_2COOH$	$1.52 \cdot 10^{5}$	9300	[66]	0.0322	[64]	0.84	[64]
H36②	$CH_3COCOBr$	$1.40 \cdot 10^{0}$	7541	[64]	0.03	[64]	0.79	[64]
H37⦸	$COBr_2$	$2.13 \cdot 10^{1}$		[66]	0.02	[64]	0.81	[64]
H38⦸	CHOBr	$7.40 \cdot 10^{1}$		[66]	0.02	[64]	1.02	[64]
H39	$BrCH_2OH$	$2.03 \cdot 10^{3}$		[66]	0.0271	as CH_3OH	1.35	[68]
H40	Br_2CHOH	$1.72 \cdot 10^{4}$		[66]	0.0271	as CH_3OH	1.32	[68]
H41	Br_3COH	$1.52 \cdot 10^{5}$		[66]	0.0271	as CH_3OH	1.33	[68]
H42	$BrCH_2OOH$	$2.53 \cdot 10^{3}$		[66]	0.006758	as CH_3OOH	1.25	[68]
H43	CH_3COCH_2Br	$1.72 \cdot 10^{2}$		[66]	0.0054	as CH_3COCH_3	0.96	[68]
H44②	I_2	$3.00 \cdot 10^{0}$	4431	[64]	0.0126	[64]	0.86	[64]
H45②	I	$8.00 \cdot 10^{-2}$		[64]	0.05	[64]	1.16	[64]
H46⦸	IO	$5.50 \cdot 10^{0}$		estimated as ClO	0.558	[64]	1.10	[64]
H47⦸	OIO	$1.00 \cdot 10^{4}$		[66]	1	[64]	1.04	[64]
H48⦸	I_2O_2	$1.00 \cdot 10^{4}$		[66]	0.123	[64]	0.80	[64]
H49	I_2O_3	$1.00 \cdot 10^{4}$		[66]	0.1	estimated	0.80	[68]
H50	I_2O_4	$1.00 \cdot 10^{4}$		[66]	0.1	estimated	0.80	[68]
H51②	HI	$2.50 \cdot 10^{0}$	9800	[64]	0.057	[64]	1.14	[64]
H52②	HOI	$4.50 \cdot 10^{2}$	5862	[64]	0.5	[64]	1.08	[64]
H53②	HIO_3	$2.10 \cdot 10^{5}$	8700	[64]	0.0126	[64]	0.98	[64]
H54②	INO_2	$2.10 \cdot 10^{5}$	8700	[64]	0.123	[64]	0.99	[64]
H55②	INO_3	$2.10 \cdot 10^{5}$	8700	[64]	0.123	[64]	0.96	[64]
H56②	ICl	$1.10 \cdot 10^{2}$	5600	[64]	0.0126	[64]	0.98	[64]
H57②	IBr	$2.40 \cdot 10^{1}$	5600	[64]	0.0126	[64]	0.88	[64]
H58②	$ICH_2CO(O_2)$	$6.69 \cdot 10^{2}$	5893	[64]	0.019	[64]	0.80	[64]
H59⦸	ICH_2COOH	$2.43 \cdot 10^{4}$		[66]	0.322	[64]	0.82	[64]
H60②	COI_2	$7.00 \cdot 10^{-2}$		[64]	0.02	[64]	0.76	[64]
H61②	CHOI	$3.00 \cdot 10^{3}$	7216	[64]	0.02	[64]	0.97	[64]

Irreversible aqueous-phase reactions implemented within the CAPRAM-HM3.0.

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A1②	$Cl + Cl \rightarrow Cl_2$	$8.75 \cdot 10^{7}$		
A2②	$Cl_2^- + Cl \rightarrow Cl_2 + Cl^-$	$2.10 \cdot 10^{9}$		
A3②	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2\ Cl^-$	$1.80 \cdot 10^{9}$		
A4②	$Cl^- + O_3 \rightarrow ClO^- + O_2$	$3.00 \cdot 10^{-3}$		
A5②	$Cl + H_2O_2 \rightarrow H^+ + Cl^- + HO_2$	$2.00 \cdot 10^{9}$		
A6⦸	$Cl_2^- + H_2O_2 \rightarrow 2\ Cl^- + H^+ + HO_2$	$6.20 \cdot 10^{5}$	3340	k_{298} after [69], E_A/R after [70]
A7②	$Cl_2^- + H_2O \rightarrow H^+ + Cl^- + ClOH^-$	$2.34 \cdot 10^{1}$		
A8②	$Cl_2^- + HO_2 \rightarrow 2\ Cl^- + H^+ + O_2$	$1.30 \cdot 10^{10}$		
A9②	$Cl_2^- + O_2^- \rightarrow 2\ Cl^- + O_2$	$6.00 \cdot 10^{9}$		
A10②	$Cl_2^- + OH \rightarrow HOCl + Cl^-$	$1.00 \cdot 10^{9}$		
A11②	$Cl_2^- + OH^- \rightarrow 2\ Cl^- + OH$	$4.00 \cdot 10^{6}$		
A12②	$Cl_3^- + HO_2 \rightarrow Cl_2^- + H^+ + Cl^- + O_2$	$1.00 \cdot 10^{9}$		
A13②	$Cl_3^- + O_2^- \rightarrow Cl_2^- + Cl^- + O_2$	$3.80 \cdot 10^{9}$		
A14②	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+ + O_2$	$1.00 \cdot 10^{9}$		
A15②	$Cl_2 + O_2^- \rightarrow Cl_2^- + O_2$	$1.00 \cdot 10^{9}$		
A16⦸	$HOCl + H_2O_2 \rightarrow H^+ + Cl^- + H_2O + O_2$	$8.17 \cdot 10^{-1}$		revised, [71]
A17⦸	$ClO^- + H_2O_2 \rightarrow Cl^- + H_2O + O_2$	$2.83 \cdot 10^{3}$	5840	revised, [71]
A18②	$HOCl + HO_2 \rightarrow Cl + H_2O + O_2$	$7.50 \cdot 10^{6}$		
A19⦸	$HOCl + O_2^- \rightarrow ClOH^- + O_2$	$7.50 \cdot 10^{6}$		product after reaction HOBr with O_2^-
A20②	$ClO^- + O_2^- \rightarrow Cl + 2\ OH^- + O_2 - H_2O$	$2.00 \cdot 10^{8}$		
A21②	$HOCl + OH \rightarrow ClO + H_2O$	$2.00 \cdot 10^{9}$		
A22②	$ClO^- + OH \rightarrow ClO + OH^-$	$8.80 \cdot 10^{9}$		
A23②	$Cl_2^- + HSO_3^- \rightarrow 2\ Cl^- + H^+ + SO_3^-$	$1.70 \cdot 10^{8}$	400	
A24②	$Cl_2^- + SO_3^{2-} \rightarrow 2\ Cl^- + SO_3^-$	$6.20 \cdot 10^{7}$		
A25②	$HOCl + SO_3^{2-} \rightarrow Cl^- + HSO_4^-$	$7.60 \cdot 10^{8}$		
A26②	$HOCl + HSO_3^- \rightarrow Cl^- + H^+ + HSO_4^{2-}$	$7.60 \cdot 10^{8}$		
A27②	$Cl^- + HSO_5^- \rightarrow HOCl + SO_4^{2-}$	$1.80 \cdot 10^{-3}$	7352	
A28②	$Cl_2^- + CH_2OHSO_3^- \rightarrow 2\ Cl^- + CH_2OHSO_3$	$5.00 \cdot 10^{5}$		

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A29②	$Cl_2^- + NO_2^- \rightarrow 2\ Cl^- + NO_2$	$6.00 \cdot 10^7$		
A30②	$Cl_2^- + Fe_2^+ \rightarrow 2\ Cl^- + Fe_3^+$	$1.00 \cdot 10^7$	3030	
A31②	$Cl_2^- + Fe_2^+ \rightarrow FeCl^{2+} + Cl^-$	$4.00 \cdot 10^6$	3490	
A32②	$Cl^- + FeO_2^+ \rightarrow Fe_3^+ + ClOH^- + OH^- - H_2O$	$1.00 \cdot 10^2$		
A33②	$Cl_2^- + Mn_2^+ \rightarrow MnCl_2^+$	$2.00 \cdot 10^7$	4090	
A34②	$MnCl_2^+ \rightarrow Cl_2^- + Mn_2^+$	$3.00 \cdot 10^5$		
A35②	$MnCl_2^+ \rightarrow 2\ Cl^- + Mn_3^+$	$2.10 \cdot 10^5$		
A36②	$Cl_2^- + Cu^+ \rightarrow 2\ Cl^- + Cu_2^+$	$1.00 \cdot 10^8$		
A37②	$Cl + CO_3^{2-} \rightarrow Cl^- + CO_3^-$	$5.00 \cdot 10^8$		
A38②	$Cl + HCO_3^- \rightarrow Cl^- + H^+ + CO_3^-$	$2.20 \cdot 10^8$		
A39②	$Cl_2^- + CO_3^{2-} \rightarrow 2\ Cl^- + CO_3^-$	$2.70 \cdot 10^6$		
A40②	$Cl_2^- + HCO_3^- \rightarrow 2\ Cl^- + H^+ + CO_3^-$	$2.70 \cdot 10^6$		
A41②	$ClNO_3 \rightarrow HOCl + HNO_3$	$1.62 \cdot 10^6$	2800	
A42②	$ClNO_3 + H^+ \rightarrow HOCl + NO_2^+$	$1.12 \cdot 10^3$	6200	
A43	$Cl^- + H_2O_2 \rightarrow ClO^- + H_2O$	$1.10 \cdot 10^{-7}$	11881	[72]
A44	$Cl^- + H_2O_2 + H^+ \rightarrow HOCl + H_2O$	$2.30 \cdot 10^{-5}$	10622	[72]
A45	$Fe^{2+} + HOCl \rightarrow Fe^{3+} + Cl^- + OH$	$1.70 \cdot 10^4$		[73]
A46	$Fe^{2+} + ClO_2 \rightarrow Fe^{3+} + ClO_2^-$	$3.00 \cdot 10^3$		[74]
A47	$Fe^{2+} + ClO_3 \rightarrow Fe^{3+} + ClO_3^-$	$7.00 \cdot 10^7$		[75]
A48	$ClO^- + O_3 \rightarrow 0.79\ Cl^- + 0.21\ ClO_2^- + 1.79\ O_2$	$1.40 \cdot 10^2$		[76]
A49	$ClO + O_3^- \rightarrow ClO^- + O_3$	$1.00 \cdot 10^9$		[77]
A50	$ClO_2 + NO_2^- \rightarrow ClO_2^- + NO_2$	$1.13 \cdot 10^2$		[74]
A51	$ClO_2 + O_3 \rightarrow ClO_3 + O_2$	$1.37 \cdot 10^3$		[74]
A52	$ClO_2 + OH \rightarrow ClO_3^- + H^+$	$4.00 \cdot 10^9$		[77]
A53	$Cl_2^- + O_3 \rightarrow ClO^- + Cl + O_2$	$9.00 \cdot 10^7$		[78], products after [79]
A54	$ClO_2 + SO_3^{2-} \rightarrow ClO_2^- + SO_3^-$	$2.70 \cdot 10^6$		[80]
A55	$ClO_2 + O_2^- \rightarrow ClO_2^- + O_2$	$3.00 \cdot 10^9$		[80]
A56	$ClO_2^- + OH \rightarrow ClO_2 + OH^-$	$6.10 \cdot 10^9$		[81]
A57	$ClO_2 \rightarrow Cl + O_2$	$6.70 \cdot 10^9$		[82]
A58	$HOCl + CH_3COCOO^- \rightarrow CH_3COOH + Cl^- + CO_2$	$2.17 \cdot 10^0$		[83]
A59	$HClO_2 + HCHO \rightarrow HCOOH + HOCl$	$1.20 \cdot 10^4$	6495	[84]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A60	$HClO_2 + HOCH_2CHO \rightarrow HOCH_2COOH + HOCl$	$4.50 \cdot 10^2$	5413	[84]
A61	$Cl_2 + NO_2^- \rightarrow ClNO_2 + Cl^-$	$2.50 \cdot 10^6$		[85]
A62	$ClNO_2 + NO_2^- \rightarrow N_2O_4 + Cl^-$	$7.97 \cdot 10^3$		[86], average
A63	$Cl + NO_2^- \rightarrow Cl^- + NO_2$	$5.00 \cdot 10^9$		[87]
A64	$Cl + HOCl \rightarrow Cl^- + ClO + H^+$	$3.00 \cdot 10^9$		[88]
A65	$Cl + ClO^- \rightarrow Cl^- + ClO$	$8.20 \cdot 10^9$		[88]
A66	$ClO^- + SO_3^{2-} \rightarrow Cl^- + SO_4^{2-}$	$2.30 \cdot 10^4$		[89]
A67	$HOCl + SO_4^- \rightarrow ClO + HSO_4^-$	$1.10 \cdot 10^7$		[90]
A68	$ClO^- + SO_4^- \rightarrow ClO + SO_4^{2-}$	$1.30 \cdot 10^9$		[90]
A69	$ClO_2^- + SO_4^- \rightarrow ClO_2 + SO_4^{2-}$	$2.05 \cdot 10^9$		[90]
A70	$HOCl + NO_3 \rightarrow ClO + HNO_3$	$4.30 \cdot 10^7$		[90]
A71	$ClO^- + NO_3 \rightarrow ClO + NO_3^-$	$3.60 \cdot 10^9$		[90]
A72	$ClO_2^- + NO_3 \rightarrow ClO_2 + NO_3^-$	$4.10 \cdot 10^9$		[90]
A73	$ClO_2^- + HSO_3^- \rightarrow OCl^- + HSO_4^-$	$5.50 \cdot 10^0$		[91]
A74	$ClO_2^- + SO_2 \rightarrow ClO^- + SO_3$	$6.26 \cdot 10^6$		[91]
A75	$2\ ClO \rightarrow Cl_2O_2$	$2.50 \cdot 10^9$		[77]
A76	$HOCl + HClO_2 \rightarrow Cl_2O_2 + H_2O$	$1.00 \cdot 10^5$		[92]
A77	$HOCl + ClO_2^- + H^+ \rightarrow Cl_2O_2 + H_2O$	$1.06 \cdot 10^6$		[93]
A78	$Cl_2O_2 + H_2O \rightarrow Cl^- + ClO_3^- + 2\ H+$	$1.80 \cdot 10^2$		[94]
A79	$2\ Cl_2O_2 \rightarrow 2\ ClO_2 + Cl_2$	$9.00 \cdot 10^2$		[95]
A80	$Cl_2O_2 + ClO_2^- \rightarrow Cl^- + 2\ ClO_2$	$5.00 \cdot 10^8$		[93]
A81	$OH + ClO_3^- \rightarrow ClO_3 + OH^-$	$1.00 \cdot 10^6$		[81]
A82	$Cl + ClO_3^- \rightarrow ClO_3 + Cl^-$	$5.00 \cdot 10^8$		[87]
A83	$ClO_3 \rightarrow ClO + O_2$	$2.00 \cdot 10^5$		estimated same as BrO_3
A84	$2\ HOCl + ClO_2^- \rightarrow ClO_3^- + Cl_2 + H_2O$	$3.25 \cdot 10^3$		[93]
A85	$Cl_2 + H_2O_2 \rightarrow 2\ H^+ + 2\ Cl^- + O_2$	$1.83 \cdot 10^2$	5387	[71]
A86	$Cl + Fe^{2+} \rightarrow Cl^- + Fe^{3+}$	$5.90 \cdot 10^9$		[96]
A87	$FeCl^{2+} + h\nu \rightarrow Cl + Fe^{2+}$	$7.59 \cdot 10^{-5}$		Absorption [97], Quantum Yield [98], TUV
A88	$Cl^- + CH_3CH_2OOH \rightarrow HOCl + CH_3COO^- + H_2O$	$1.47 \cdot 10^{-5}$		[99]
A89②	$Cl_2^- + CH_3OOH \rightarrow 2\ Cl^- + H^+ + CH_3OO$	$5.00 \cdot 10^4$	3340	
A90②	$Cl + CH_3OH \rightarrow Cl^- + H^+ + CH_2OH$	$1.00 \cdot 10^9$	4089	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A91②	$Cl_2^- + CH_3OH \rightarrow 2\ Cl^- + H^+ + CH_2OH$	$5.10 \cdot 10^4$	5533	
A92②	$Cl + C_2H_5OH \rightarrow Cl^- + H^+ + CH_3CHOH$	$1.60 \cdot 10^9$		
A93②	$Cl_2^- + C_2H_5OH \rightarrow 2\ Cl^- + H^+ + CH_3CHOH$	$1.20 \cdot 10^5$		
A94②	$Cl + C_3H_7OH \rightarrow Cl^- + H^+ + C2H_5CHOH$	$2.20 \cdot 10^9$	2285	
A95②	$Cl_2^- + C_3H_7OH \rightarrow 2\ Cl^- + H^+ + C2H_5CHOH$	$1.00 \cdot 10^5$		
A96②	$Cl + CH_3CHOHCH_3 \rightarrow Cl^- + H^+ + CH_3COHCH_3$	$3.20 \cdot 10^9$	2766	
A97②	$Cl_2^- + CH_3CHOHCH_3 \rightarrow 2\ Cl^- + H^+ + CH_3COHCH_3$	$1.90 \cdot 10^5$		
A98②	$Cl + CH_2(OH)_2 \rightarrow Cl^- + H^+ + CH(OH)_2$	$1.40 \cdot 10^9$	3127	
A99②	$Cl_2^- + CH_2(OH)_2 \rightarrow 2\ Cl^- + H^+ + CH(OH)_2$	$3.60 \cdot 10^4$	4330	
A100②	$Cl + CH_3CHO \rightarrow Cl^- + H^+ + CH_3CO$	$6.00 \cdot 10^8$	1928	
A101②	$Cl + CH_3CH(OH)_2 \rightarrow Cl^- + H^+ + CH_3C(OH)_2$	$6.00 \cdot 10^8$	1928	
A102②	$Cl_2^- + CH_3CHO \rightarrow 2\ Cl^- + H^+ + CH_3CO$	$4.00 \cdot 10^4$		
A103②	$Cl_2^- + CH_3CH(OH)_2 \rightarrow 2\ Cl^- + H^+ + CH_3C(OH)_2$	$4.00 \cdot 10^4$		
A104②	$Cl + C_2H_5CHO \rightarrow Cl^- + H^+ + C_2H_5CO$	$7.50 \cdot 10^8$	1566	
A105②	$Cl + C_2H_5CH(OH)_2 \rightarrow Cl^- + H^+ + C_2H_5C(OH)_2$	$7.50 \cdot 10^8$	1566	
A106②	$Cl + C_3H_7CHO \rightarrow Cl^- + H^+ + C_3H_7CO$	$2.20 \cdot 10^9$	1686	
A107②	$Cl + C_3H_7CH(OH)_2 \rightarrow Cl^- + H^+ + C_3H_7C(OH)_2$	$1.10 \cdot 10^9$	1686	
A108②	$Cl + CH_3COCH_3 \rightarrow Cl^- + H^+ + CH_3COCH_2$	$7.80 \cdot 10^7$		
A109②	$Cl_2^- + CH_3COCH_3 \rightarrow 2\ Cl^- + H^+ + CH_3COCH_2$	$1.40 \cdot 10^3$		
A110②	$Cl + HCOOH \rightarrow Cl^- + H^+ + COOH$	$2.80 \cdot 10^9$	2405	
A111②	$Cl + HCOO^- \rightarrow Cl^- + COOH$	$4.20 \cdot 10^9$	1924	
A112②	$Cl_2^- + HCOOH \rightarrow 2\ Cl^- + H^+ + COOH$	$8.00 \cdot 10^4$	4450	
A113②	$Cl_2^- + HCOO^- \rightarrow 2\ Cl^- + COOH$	$1.30 \cdot 10^6$	4930	
A114②	$Cl + CH_3COOH \rightarrow Cl^- + H^+ + CH_2COOH$	$1.00 \cdot 10^8$	1684	
A115②	$Cl + CH_3COO^- \rightarrow Cl^- + CH_3 + CO_2$	$3.70 \cdot 10^9$	4930	
A116②	$Cl_2^- + CH_3COOH \rightarrow 2\ Cl^- + H^+ + CH_2COOH$	$1.50 \cdot 10^3$	4800	
A117②	$Cl_2^- + CH_3COO^- \rightarrow 2\ Cl^- + CH_3 + CO_2$	$2.60 \cdot 10^5$	5292	
A118②	$Cl + C_2H_5COOH \rightarrow Cl^- + H^+ + CH_3CHCOOH$	$1.20 \cdot 10^9$	5292	
A119②	$Cl + C_2H_5COO^- \rightarrow Cl^- + CH_3CHCOO^-$	$1.20 \cdot 10^9$		
A120②	$Cl_2^- + HC_2O_4^- \rightarrow 2\ Cl^- + H^+ + C_2O_4^-$	$1.30 \cdot 10^6$		
A121②	$Cl_2^- + C_2O_4^{2-} \rightarrow 2\ Cl^- + C_2O_4^-$	$4.00 \cdot 10^6$		

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A122②	$Cl_2^- + CH(OH)_2CH(OH)_2 \rightarrow 2\ Cl^- + H^+ + C(OH)_2CH(OH)_2$	$4.00 \cdot 10^4$		
A123②	$Cl_2^- + CH(OH)_2COOH \rightarrow 2\ Cl^- + H^+ + C(OH)_2COOH$	$4.00 \cdot 10^4$		
A124②	$CH_2ClC(OH)_2O_2 \rightarrow CH_2ClCOOH + HO_2$	$1.00 \cdot 10^3$		
A125②	$CH_2ClC(OH)_2O_2 \rightarrow CH_2ClCOO^- + H^+ + O_2^-$	$1.00 \cdot 10^5$		
A126②	$CH_3COCClO + H_2O \rightarrow CH_3COCOOH + H^+ + Cl^-$	$3.50 \cdot 10^2$		
A127②	$CHOCl \rightarrow CO + H^+ + Cl^-$	$1.00 \cdot 10^4$		
A128②	$CHOCl + OH^- \rightarrow HCOO^- + H^+ + Cl^-$	$2.50 \cdot 10^4$		
A129②	$COCl_2 + H_2O \rightarrow ClCOOH + H^+ + Cl^-$	$1.00 \cdot 10^1$		
A130②	$COCl_2 + OH^- \rightarrow ClCOOH + Cl^-$	$2.80 \cdot 10^4$		
A131②	$ClCOOH \rightarrow CO_2 + H^+ + Cl^-$	$1.00 \cdot 10^5$		
A132	$CH_3CClO + H_2O \rightarrow CH_3COOH + Cl^- + H^+$	$3.50 \cdot 10^2$		[100]
A133	$ClCH_2CClO + H_2O \rightarrow ClCH_2COOH + Cl^- + H^+$	$5.50 \cdot 10^0$		[100]
A134	$ClCH_2CH_2OH + OH \rightarrow ClCH_2CH(OH)O_2 + H_2O$	$8.36 \cdot 10^8$	1067	[101]
A135	$ClCH_2CH(OH)O_2 \rightarrow ClCH_2CHO$	$2.00 \cdot 10^2$		[102]
A136	$2\ ClCH_2CH(OH)O_2 \rightarrow ClCH_2COOH + H_2O_2$	$7.30 \cdot 10^8$		[102]
A137②	$Br + Br \rightarrow Br_2$	$1.00 \cdot 10^9$		
A138⦸	$Br_2^- + Br_2^- \rightarrow Br_3^- + Br^-$	$2.04 \cdot 10^9$		revised
A139②	$Br^- + O_3 \rightarrow BrO^- + O_2$	$2.10 \cdot 10^2$	4450	
A140②	$Br + HO_2 \rightarrow H^+ + Br^- + O_2$	$1.60 \cdot 10^8$		
A141②	$Br + H_2O_2 \rightarrow H^+ + Br^- + HO_2$	$4.00 \cdot 10^9$		
A142②	$Br_2 + HO_2 \rightarrow H^+ + Br^- + O_2$	$1.10 \cdot 10^8$		
A143②	$Br_2 + O_2^- \rightarrow Br_2^- + O_2$	$5.60 \cdot 10^9$		
A144②	$Br_2 + H_2O_2 \rightarrow 2\ H^+ + 2\ Br^- + O_2$	$1.30 \cdot 10^3$		
A145②	$Br_2^- + OH \rightarrow Br^- + HOBr$	$1.00 \cdot 10^9$		
A146②	$Br_2^- + OH^- \rightarrow 2\ Br^- + OH$	$1.10 \cdot 10^4$		
A147②	$Br_2^-\ HO_2 \rightarrow 2\ Br^- + H^+ + O_2$	$4.40 \cdot 10^9$		
A148②	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 - H^+$	$4.40 \cdot 10^9$		
A149②	$Br_2^- + O_2^- \rightarrow 2\ Br^- + O_2$	$1.70 \cdot 10^8$		
A150②	$Br_2^- + H_2O_2 \rightarrow 2\ Br^- + H^+ + HO_2$	$1.00 \cdot 10^5$		
A151②	$Br_3^- + HO_2 \rightarrow Br_2^- + H^+ + Br^- + O_2$	$1.00 \cdot 10^7$		
A152②	$Br_3^- + O_2^- \rightarrow Br_2^- + Br^- + O_2$	$3.80 \cdot 10^9$		

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A153②	$BrO + BrO \rightarrow BrO_2^- + BrO^- + 2\ H^+ - H_2O$	$2.80 \cdot 10^9$		
A154②	$BrO_2^- + BrO \rightarrow BrO_2 + BrO^-$	$4.00 \cdot 10^8$		
A155②	$Br_2^- + BrO_2^- \rightarrow 2\ Br^- + BrO_2$	$8.00 \cdot 10^7$		
A156②	$BrO_2^- + OH \rightarrow BrO_2 + OH^-$	$1.80 \cdot 10^9$		
A157②	$HOBr + OH \rightarrow BrO + H_2O$	$2.00 \cdot 10^9$		
A158②	$BrO^- + OH \rightarrow BrO + OH^-$	$4.50 \cdot 10^9$		
A159②	$HOBr + HO_2 \rightarrow Br + H_2O + O_2$	$1.00 \cdot 10^9$		
A160⦸	$HOBr + O_2^- \rightarrow BrOH^- + O_2$	$3.50 \cdot 10^9$		product [103]
A161②	$BrO^- + O_2^- \rightarrow Br + 2\ OH^- + O_2 - H_2O$	$2.00 \cdot 10^8$		
A162②	$HOBr + H_2O_2 \rightarrow H^+ + Br^- + H_2O + O_2$	$3.50 \cdot 10^6$		
A163②	$BrO^- + H_2O_2 \rightarrow Br^- + H_2O + O_2$	$2.00 \cdot 10^5$		
A164②	$Br_2^- + HSO_3^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	$5.00 \cdot 10^7$	780	
A165②	$Br_2^- + SO_3^{2-} \rightarrow 2\ Br^- + SO_3^-$	$3.30 \cdot 10^7$	650	
A166②	$Br^- + SO_4^- \rightarrow Br + SO_4^{2-}$	$2.10 \cdot 10^9$		
A167②	$HOBr + SO_3^{2-} \rightarrow Br^- + HSO_4^-$	$5.00 \cdot 10^9$		
A168②	$HOBr + HSO_3^- \rightarrow H+ + Br^- + HSO_4^-$	$5.00 \cdot 10^9$		
A169②	$Br^- + HSO_5^- \rightarrow HOBr + SO_4^{2-}$	$1.00 \cdot 10^0$	5338	
A170②	$Br_2^- + CH_2OHSO_3^- \rightarrow 2\ Br^- + CH_2OHSO_3$	$5.00 \cdot 10^4$		
A171②	$Br^- + NO_3 \rightarrow Br + NO_3^-$	$3.80 \cdot 10^9$		
A172②	$Br_2^- + NO_2^- \rightarrow 2\ Br^- + NO_2$	$1.20 \cdot 10^7$	1720	
A173②	$Br^- + NO_2^+ \rightarrow BrNO_2$	$1.00 \cdot 10^{10}$		
A174②	$Br_2^- + Fe^{2+} \rightarrow 2\ Br^- + Fe^{3+}$	$3.60 \cdot 10^6$	3330	
A175②	$MnBr_2^+ \rightarrow 2\ Br- + Mn^{3+}$	$2.20 \cdot 10^5$		
A176②	$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	$6.30 \cdot 10^6$	4330	
A177②	$MnBr_2^+ \rightarrow Br_2^- + Mn^{2+}$	$3.00 \cdot 10^5$		
A178②	$Br_2^- + Cu^+ \rightarrow 2\ Br^- + Cu^{2+}$	$3.60 \cdot 10^6$		
A179②	$Br + HCO_3^- \rightarrow H^+ + Br^- + CO_3^-$	$1.00 \cdot 10^6$		
A180②	$Br_2^- + CO_3^{2-} \rightarrow 2\ Br^- + CO_3^-$	$1.10 \cdot 10^5$		
A181②	$Br_2^- + HCO_3^- \rightarrow 2\ Br^- + H^+ + CO_3^-$	$1.10 \cdot 10^5$		
A182②	$BrNO_3 \rightarrow HOBr + HNO_3$	$1.00 \cdot 10^9$		
A183②	$BrNO_3 + H^+ \rightarrow HOBr + NO_2^+$	$1.12 \cdot 10^3$	6200	

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A184	$Br^- + H_2O_2 \rightarrow BrO^- + H_2O$	$1.10 \cdot 10^{-1}$	6746	72
A185	$Br^- + H_2O_2 + H^+ \rightarrow HOBr + H_2O$	$5.00 \cdot 10^{-5}$	10441	72
A186	$BrO + O_3^- \rightarrow BrO^- + O_3$	$1.50 \cdot 10^{9}$		104
A187	$HOBr + O_3 \rightarrow BrO_2^- + H^+ + O_2$	$1.30 \cdot 10^{-2}$		76
A188	$BrO^- + O_3 \rightarrow 0.77\ Br^- + 0.23\ BrO_2^- + 1.77\ O_2$	$4.30 \cdot 10^{2}$		76
A189	$BrO_2 + NO_2^- \rightarrow BrO_2^- + NO_2$	$2.00 \cdot 10^{6}$		80
A190	$BrO_2 + SO_3^{2-} \rightarrow BrO_2^- + SO_3^-$	$9.50 \cdot 10^{8}$		80
A191	$BrO_3^- + SO_4^- \rightarrow BrO_3 + SO_4^{2-}$	$1.40 \cdot 10^{6}$		105
A192	$BrO_3 \rightarrow BrO + O_2$	$2.00 \cdot 10^{5}$		105
A193	$BrNO_2 + NO_2^- \rightarrow N_2O_4 + Br^-$	$1.27 \cdot 10^{4}$		85
A194	$Br + O_3 \rightarrow BrO + O_2$	$1.50 \cdot 10^{8}$		106
A195	$BrO^- + SO_3^{2-} \rightarrow Br^- + SO_4^{2-}$	$1.00 \cdot 10^{8}$		107
A196	$2\ HOBr + CO_3^{2-} \rightarrow BrO_2^- + Br^- + HCO_3^- + H^+$	$3.30 \cdot 10^{-1}$		108
A197	$2\ HOBr + OH^- \rightarrow BrO_2^- + Br^- + H^+ + H_2O$	$1.50 \cdot 10^{1}$		108
A198	$BrO^- + CO_3^- \rightarrow BrO + CO_3^{2-}$	$4.30 \cdot 10^{7}$		109
A199	$BrO^- + Br_2^- \rightarrow BrO + 2\ Br^-$	$8.00 \cdot 10^{7}$		109
A200	$BrO_2^- + CO_3^- \rightarrow BrO_2 + CO_3^{2-}$	$1.10 \cdot 10^{8}$		109
A201	$BrO_2 + OH \rightarrow BrO_3^- + H^+$	$2.00 \cdot 10^{9}$		110
A202	$BrO_2 + Mn^{2+} \rightarrow BrO_2^- + Mn^{3+}$	$1.50 \cdot 10^{6}$		110
A203	$Br_2O_4 + Mn^{2+} \rightarrow BrO_2 + BrO_2^- + Mn^{3+}$	$1.00 \cdot 10^{8}$		110
A204	$BrO_3^- + SO_2 \rightarrow BrO_2^- + SO_4^{2-} + 2\ H^+$	$8.50 \cdot 10^{0}$		111
A205	$BrO_3^- + HSO_3^- \rightarrow BrO_2^- + SO_4^{2-} + H^+$	$2.70 \cdot 10^{-2}$		111
A206	$HBrO_2 + BrO_2^- \rightarrow HOBr + BrO_3^-$	$3.91 \cdot 10^{1}$		112
A207	$HOBr + BrO_2^- \rightarrow Br^- + BrO_3^- + H^+$	$8.00 \cdot 10^{-3}$		108
A208	$BrO_3^- + OH \rightarrow BrO_3 + OH^-$	$5.00 \cdot 10^{6}$		113
A209②	$Br_2^- + Cl_2^- \rightarrow Br_2 + 2\ Cl^-$	$4.00 \cdot 10^{9}$		
A210②	$Br^- + HOCl + H^+ \rightarrow BrCl + H_2O$	$1.30 \cdot 10^{6}$		
A211②	$Br^- + ClO^- \rightarrow BrCl + OH^- - H^+$	$3.65 \cdot 10^{10}$		
A212②	$Br^- + ClNO_2 \rightarrow BrCl + NO_2^-$	$5.00 \cdot 10^{6}$		
A213②	$BrNO_2 + Cl^- \rightarrow BrCl + NO_2^-$	$1.00 \cdot 10^{1}$		
A214	$ClO_2^- + Br_2^- \rightarrow 2\ Br^- + ClO_2$	$2.00 \cdot 10^{7}$		80

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A215	$BrO_2^- + HOCl \rightarrow$ 0.85 ClO_3^- + 0.93 HOBr + 0.08 ClO_2^- + 0.07 BrO_3^- + 0.92 Cl^- + 0.92 H^+ - 0.85 HOCl	$1.60 \cdot 10^2$		[114]
A216	$BrOCl(OH)_2 + H^+ \rightarrow HOBr + HClO_2 + H^+$	$5.35 \cdot 10^2$		[115]
A217	$HClO_2 + Br^- \rightarrow HOCl + BrO^-$	$1.00 \cdot 10^{-3}$		[115]
A218	$Br + ClO_2^- \rightarrow ClO_2 + Br^-$	$2.30 \cdot 10^8$		[116]
A219	$Br_2^- + ClO_2^- \rightarrow ClO_2 + 2\ Br^-$	$4.00 \cdot 10^6$		[116]
A220	$HOCl + Br^- + ClCH_2COOH \rightarrow BrCl + ClCH_2COO^- + H_2O$	$6.11 \cdot 10^4$		[117]
A221	$HOCl + Br^- + CH_3COOH \rightarrow BrCl + CH_3COO^- + H_2O$	$2.09 \cdot 10^4$		[117]
A222	$HOCl + Br^- \rightarrow BrCl + OH^-$	$1.55 \cdot 10^3$		[117]
A223	$ClO^- + Br^- + HCO_3^- \rightarrow BrCl + OH^- + CO_3^{2-}$	$1.25 \cdot 10^2$		[117]
A224	$ClO^- + Br^- \rightarrow BrCl + 2\ OH^- - H_2O$	$8.88 \cdot 10^{-4}$		[117]
A225	$ClO_2 + BrO_2 + H_2O \rightarrow BrO_2^- + ClO_3^- + 2\ H^+$	$2.00 \cdot 10^4$		[118]
A226	$ClO_2 + BrO_2 + OH^- \rightarrow BrO_2^- + ClO_3^- + H^+$	$1.25 \cdot 10^8$		[118]
A227	$ClO_2 + BrO_2 + SO_4^{2-} \rightarrow BrO_2^- + ClO_3^- + SO_4^{2-} + H_2O - 2\ OH^-$	$3.60 \cdot 10^7$		[118]
A228	$ClO_2 + BrO_2 + CH_3COO^- \rightarrow BrO_2^- + ClO_3^- + CH_3COO^- + H_2O - 2\ OH^-$	$4.40 \cdot 10^7$		[118]
A229	$ClO_2 + BrO_2 + Cl^- \rightarrow BrO_2\text{-} + ClO_3^- + Cl^- + H_2O - 2\ OH^-$	$1.28 \cdot 10^8$		[118]
A230	$ClO_2 + BrO_2 + CO_3^{2-} \rightarrow BrO_2\text{-} + ClO_3^- + CO_3^{2-} + H_2O - 2\ OH^-$	$1.49 \cdot 10^8$		[118]
A231	$ClO_2 + BrO_2 + ClO_2^- \rightarrow BrO_2^- + ClO_3^- + ClO_2^- + H_2O - 2\ OH^-$	$2.20 \cdot 10^8$		[118]
A232	$ClO_2 + BrO_2 + BrO_2^- \rightarrow BrO_2^- + ClO_3^- + BrO_2^- + H_2O - 2\ OH^-$	$2.30 \cdot 10^8$		[118]
A233	$ClO_2 + BrO_2 + Br^- \rightarrow BrO_2^- + ClO_3^- + Br^- + H_2O - 2\ OH^-$	$2.89 \cdot 10^8$		[118]
A234	$Br^- + CH_3CH_2OOH \rightarrow HOBr + CH_3COO^- + H_2O$	$2.40 \cdot 10^{-1}$		[99]
A235②	$Br_2^- + CH_3OOH \rightarrow 2\ Br^- + H^+ + CH_3OO$	$1.00 \cdot 10^5$		
A236②	$Br + CH_3OH \rightarrow Br^- + H^+ + CH_2OH$	$4.10 \cdot 10^4$	3368	
A237②	$Br_2^- + CH_3OH \rightarrow 2\ Br^- + H^+ + CH_2OH$	$1.00 \cdot 10^3$		
A238②	$Br + C_2H_5OH \rightarrow Br^- + H^+ + CH_3CHOH$	$8.20 \cdot 10^5$	2285	
A239②	$Br_2^- + C_2H_5OH \rightarrow 2\ Br^- + H^+ + CH_3CHOH$	$3.80 \cdot 10^3$		
A240②	$Br + C_3H_7OH \rightarrow Br^- + H^+ + C_2H_5CHOH$	$3.80 \cdot 10^5$	1564	
A241②	$Br + CH_3CHOHCH_3 \rightarrow Br^- + H^+ + CH_3COHCH_3$	$1.80 \cdot 10^6$	3127	
A242②	$Br + CH_2(OH)_2 \rightarrow Br^- + H^+ + CH(OH)_2$	$3.00 \cdot 10^5$	3608	
A243②	$Br_2^- + CH_2(OH)_2 \rightarrow 2\ Br^- + H^+ + CH(OH)_2$	$3.00 \cdot 10^3$		

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A244②	$Br + CH_3CHO \rightarrow Br^- + H^+ + CH_2CHO$	$1.75 \cdot 10^7$	1804	
A245②	$Br + CH_3CH(OH)_2 \rightarrow Br^- + H^+ + CH_3C(OH)_2$	$1.75 \cdot 10^7$	1804	
A246②	$Br_2^- + CH_3CHO \rightarrow 2\ Br^- + H^+ + CH_2CHO$	$2.15 \cdot 10^5$	2526	
A247②	$Br_2^- + CH_3CH(OH)_2 \rightarrow 2\ Br^- + H^+ + CH_3C(OH)_2$	$2.15 \cdot 10^5$	2526	
A248②	$Br + C_2H_5CHO \rightarrow Br^- + H^+ + C_2H_5CO$	$2.85 \cdot 10^7$	842	
A249②	$Br + C_2H_5CH(OH)_2 \rightarrow Br^- + H^+ + C_2H_5C(OH)_2$	$2.85 \cdot 10^7$	842	
A250②	$Br_2^- + C_2H_5CHO \rightarrow 2\ Br^- + H^+ + C_2H_5CO$	$4.95 \cdot 10^5$	3614	
A251②	$Br_2^- + C_2H_5CH(OH)_2 \rightarrow 2\ Br^- + H^+ + C_2H_5C(OH)_2$	$4.95 \cdot 10^5$	3614	
A252②	$Br + C_3H_7CHO \rightarrow Br^- + H^+ + C_3H_7CO$	$6.67 \cdot 10^7$	1203	
A253②	$Br + C_3H_7CH(OH)_2 \rightarrow Br^- + H^+ + C_3H_7C(OH)_2$	$3.33 \cdot 10^7$	1203	
A254②	$Br_2^- + C_3H_7CHO \rightarrow 2\ Br^- + H^+ + C_3H_7CO$	$2.60 \cdot 10^5$	2289	
A255②	$Br_2^- + C_3H_7CH(OH)_2 \rightarrow 2\ Br^- + H^+ + C_3H_7C(OH)_2$	$1.30 \cdot 10^5$	2289	
A256②	$Br + HCOOH \rightarrow Br^- + H^+ + COOH$	$7.70 \cdot 10^5$	2288	
A257②	$Br + HCOO^- \rightarrow Br^- + COOH$	$4.60 \cdot 10^8$		
A258②	$Br_2^- + HCOOH \rightarrow 2\ Br^- + H^+ + COOH$	$4.00 \cdot 10^3$		
A259②	$Br_2^- + HCOO^- \rightarrow 2\ Br^- + COOH$	$4.90 \cdot 10^3$		
A260②	$Br_2^- + CH_3COOH \rightarrow 2\ Br^- + H^+ + CH_2COOH$	$1.00 \cdot 10^1$		
A261②	$Br_2^- + CH_3COO^- \rightarrow 2\ Br^- + CH_3 + CO_2$	$1.00 \cdot 10^2$		
A262②	$Br_2^- + HC_2O_4^- \rightarrow 2\ Br^- + H^+ + C_2O_4^-$	$3.70 \cdot 10^3$		
A263②	$Br_2^- + C_2O_4^{2-} \rightarrow 2\ Br^- + C_2O_4^-$	$1.10 \cdot 10^4$		
A264②	$Br_2^- + CH(OH)_2CH(OH)_2 \rightarrow 2\ Br^- + H^+ + C(OH)_2CH(OH)_2$	$5.00 \cdot 10^2$		
A265②	$Br_2^- + CH(OH)_2COOH \rightarrow 2\ Br^- + H^+ + C(OH)_2COOH$	$5.00 \cdot 10^2$		
A266	$HOBr + HCOO^- \rightarrow Br^- + CO_2 + H_2O$	$1.04 \cdot 10^0$		119
A267	$Br_2 + HCOO^- \rightarrow 2\ Br^- + CO_2 + H^+$	$2.02 \cdot 10^1$		119
A268	$HOBr + C_2O_4H_2 \rightarrow Br^- + 2\ CO_2 + H^+$	$1.70 \cdot 10^1$		120
A269	$HBrO_2 + C_2O_4H_2 \rightarrow HOBr + 2\ CO_2 + H^+$	$4.20 \cdot 10^0$		120
A270	$BrO_3^- + C_2O_4H_2 \rightarrow BrO_2^- + 2\ CO_2 + H_2O$	$7.47 \cdot 10^{-4}$		120
A271②	$CH_2BrC(OH)_2O_2 \rightarrow CH_2BrCOOH + HO_2$	$1.00 \cdot 10^3$		
A272②	$CH_2BrC(OH)_2O_2 \rightarrow CH_2BrCOO^- + H^+ + O_2^-$	$1.00 \cdot 10^5$		
A273②	$CH_3COCBrO + H_2O \rightarrow CH_3COCOOH + H^+ + Br^-$	$3.50 \cdot 10^2$		
A274②	$CHOBr \rightarrow CO + H^+ + Br^-$	$1.00 \cdot 10^4$		

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A275②	$CHOBr + OH^- \rightarrow HCOO^- + H^+ + Br^-$	$2.50 \cdot 10^4$		
A276②	$COBr_2 + H_2O \rightarrow BrCOOH + H^+ + Br^-$	$1.00 \cdot 10^1$		
A277②	$COBr_2 + OH^- \rightarrow BrCOOH + Br^-$	$2.80 \cdot 10^4$		
A278②	$BrCOOH \rightarrow CO_2 + H^+ + Br^-$	$1.00 \cdot 10^5$		
A279②	$I + I \rightarrow I_2$	$1.10 \cdot 10^{10}$		
A280②	$I + I_2^- \rightarrow I_3^-$	$6.50 \cdot 10^9$		
A281②	$I_2^- + I_2^- \rightarrow I_3^- + I^-$	$2.50 \cdot 10^9$		
A282②	$I^- + O_3 \rightarrow HOI + O_2$	$2.17 \cdot 10^9$	8790	
A283②	$I_2 + HO_2 \rightarrow I_2^- + H^+ + O_2$	$6.00 \cdot 10^9$		
A284②	$I_2 + O_2^- \rightarrow I_2^- + O_2$	$6.00 \cdot 10^9$		
A285②	$I_3^- + HO_2 \rightarrow I_2^- + H^+ + I^- + O_2$	$2.50 \cdot 10^8$		
A286②	$I_3^- + O_2^- \rightarrow I_2^- + I^- + O_2$	$2.50 \cdot 10^8$		
A287②	$HIO_2 + H_2O_2 \rightarrow H^+ + IO_3^- + H_2O$	$6.00 \cdot 10^1$		
A288②	$IO_2^- + H_2O_2 \rightarrow IO_3^- + H_2O$	$6.00 \cdot 10^1$		
A289②	$IO + IO \rightarrow HOI + HIO_2 - H_2O$	$1.50 \cdot 10^9$		
A290⦸	$I_2 + HSO_3^- \rightarrow 2\ H^+ + 2\ I^- + HSO_4^- - H_2O$	$1.70 \cdot 10^9$		value from [121]
A291②	$HOI + SO_3^{2-} \rightarrow I^- + HSO_4^-$	$5.00 \cdot 10^9$		
A292②	$HOI + HSO_3^- \rightarrow H^+ + I^- + HSO_4^-$	$5.00 \cdot 10^9$		
A293②	$INO_3 \rightarrow HOI + HNO_3$	$1.62 \cdot 10^6$	2800	
A294②	$INO_3 + H^+ \rightarrow HOI + NO_2^+$	$1.12 \cdot 10^3$	6200	
A295	$I^- + H_2O_2 \rightarrow IO^- + H_2O$	$1.40 \cdot 10^{-2}$	8407	[72]
A296	$I^- + H_2O_2 + H^+ \rightarrow HOI + H_2O$	$9.95 \cdot 10^0$	5261	[72]
A297	$I_3^- + HSO_3^- \rightarrow HSO_4^- + 3\ I^- + 3\ H^+ - H_2O$	$1.50 \cdot 10^7$		[121]
A298	$I_2 + SO_3^{2-} \rightarrow SO_4^{2-} + 2\ I^- + 2\ H^+ - H_2O$	$3.10 \cdot 10^9$		[121]
A299	$I_3^- + SO_3^{2-} \rightarrow SO_4^{2-} + 3\ I^- + 2\ H^+ - H_2O$	$2.90 \cdot 10^8$		[121]
A300	$I^- + OH \rightarrow IOH^-$	$1.60 \cdot 10^{10}$		[122]
A301	$I^- + NO_3 \rightarrow I + NO_3^-$	$4.60 \cdot 10^9$		[123]
A302	$HOI + O_3 \rightarrow HIO_2 + O_2$	$3.60 \cdot 10^4$		[124]
A303	$IO^- + O_3 \rightarrow IO_2^- + O_2$	$1.60 \cdot 10^6$		[124]
A304	$HOI + OH \rightarrow IO + H_2O$	$7.00 \cdot 10^9$		[125]
A305	$I_2^- + HOI \rightarrow IO + 2\ I^- + H+$	$1.00 \cdot 10^5$		[126]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A306	$HOI + H_2O_2 \rightarrow I^- + H^+ + O_2 + H_2O$	$3.70 \cdot 10^1$		[127]
A307	$I_2O_2 + H^+ \rightarrow HIO_2 + HOI + H^+ - H_2O$	$3.20 \cdot 10^4$		[128]
A308	$2\ IO_2^- \rightarrow IO_3^- + IO^-$	$1.03 \cdot 10^2$		[129]
A309	$IO_3^- + OH \rightarrow IO_3 + OH^-$	$1.08 \cdot 10^5$		[130]
A310	$IO_3 \rightarrow IO + O_2$	$2.00 \cdot 10^5$		estimated same as for BrO_3
A311	$IO_3^- + HSO_3^- + H^+ \rightarrow HIO_2 + SO_4^{2-} + H^+$	$3.97 \cdot 10^3$		[131]
A312	$IO_3^- + HSO_3^- \rightarrow HIO_2 + SO_4^{2-}$	$1.46 \cdot 10^{-1}$		[131]
A313②	$I^- + ICl \rightarrow I_2 + Cl^-$	$1.10 \cdot 10^9$		
A314②	$I^- + HOCl + H^+ \rightarrow ICl + H_2O$	$3.50 \cdot 10^{11}$		
A315②	$I^- + HOBr \rightarrow IBr + OH^-$	$5.00 \cdot 10^9$		
A316②	$HOI + Cl_2 \rightarrow HIO_2 + 2\ H^+ + 2\ Cl^- - H_2O$	$1.00 \cdot 10^6$		
A317②	$HOI + HOCl \rightarrow HIO_2 + H^+ + Cl^-$	$5.00 \cdot 10^5$		
A318⦸	$HOI + HOBr \rightarrow HIO_2 + H^+ + Br^-$	$1.00 \cdot 10^0$		revised, [132]
A319②	$HIO_2 + HOCl \rightarrow IO_3^- + Cl^- + 2\ H^+$	$1.50 \cdot 10^3$		
A320②	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	$1.50 \cdot 10^3$		
A321②	$HIO_2 + HOBr \rightarrow IO_3^- + Br^- + 2\ H^+$	$1.00 \cdot 10^6$		
A322②	$IO_2^- + HOBr \rightarrow IO_3^- + Br^- + H^+$	$1.00 \cdot 10^6$		
A323	$IO^- + HOBr \rightarrow IO_2^- + H^+ + Br^-$	$1.90 \cdot 10^6$		[132]
A324	$IO^- + BrO^- \rightarrow IO_2^- + Br\text{-}$	$1.80 \cdot 10^3$		[132]
A325	$ClO_2 + I^- \rightarrow ClO_2^- + I$	$1.40 \cdot 10^3$		[74]
A326	$BrO_3^- + I^- + 2\ H^+ \rightarrow HBrO_2 + HOI$	$4.43 \cdot 10^1$		[133]
A327	$BrO_3^- + IBr \rightarrow IO_3^- + Br^- + HOBr + H^+$	$8.00 \cdot 10^{-4}$		[134]
A328	$HClO_2 + I^- \rightarrow IO^- + HOCl$	$5.00 \cdot 10^0$		[135]
A329	$HClO_2 + HOI \rightarrow HIO_2 + HOCl$	$6.00 \cdot 10^7$		[135]
A330	$HBrO_2 + HOI \rightarrow HIO_2 + HOBr$	$6.00 \cdot 10^7$		[136], after $HClO_2$ reaction rate
A331	$BrO^- + I^- + H_2O \rightarrow IBr + 2\ OH^-$	$6.80 \cdot 10^5$		[107]
A332	$ICl + OH^- \rightarrow HOI + Cl^-$	$4.50 \cdot 10^9$		[137]
A333	$ICl + CO_3^{2-} \rightarrow HOI + Cl^- + HCO_3^- - H_2O$	$1.40 \cdot 10^9$		[137]
A334	$IBr + OH^- \rightarrow HOI + Br^-$	$6.00 \cdot 10^9$		[138]
A335	$IBr + CO_3^{2-} \rightarrow HOI + Br^- + HCO_3^- - H_2O$	$3.50 \cdot 10^9$		[138]
A336	$ClO^- + I^- + HCO_3^- \rightarrow ICl + 2\ OH^- + HCO_3^- - H_2O$	$9.40 \cdot 10^6$		[139]

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	k_{298}	E_A/R	Reference
A337	$ClO^- + HOI \rightarrow HIO_2 + Cl^-$	$5.20 \cdot 10^1$		[124]
A338	$I^- + CH_3CH_2OOH \rightarrow HOI + CH_3COO^- + H_2O$	$4.22 \cdot 10^2$		[140]
A339②	$CH_2IC(OH)_2O_2 \rightarrow CH_2ICOOH + HO_2$	$1.00 \cdot 10^3$		
A340②	$CH_2IC(OH)_2O_2 \rightarrow CH_2ICOO^- + H^+ + O_2^-$	$1.00 \cdot 10^5$		
A341②	$CHOI \rightarrow CO + H^+ + I^-$	$1.00 \cdot 10^4$		
A342②	$CHOI + OH^- \rightarrow HCOO^- + H^+ + I^-$	$2.50 \cdot 10^4$		
A343②	$COI_2 + H_2O \rightarrow ICOOH + H^+ + I^-$	$1.00 \cdot 10^1$		
A344②	$COI_2 + OH^- \rightarrow ICOOH + I^-$	$2.80 \cdot 10^4$		
A345②	$ICOOH \rightarrow CO_2 + H^+ + I^-$	$1.00 \cdot 10^5$		
A346	$HOI + CH_2{=}CHCOOH + H^+ \rightarrow HOCH_2CH(I)COOH + H^+$	$8.07 \cdot 10^2$		[89]
A347	$I_2 + HOOCCH_2COOH \rightarrow HOOCCH(I)COOH + I^- + H^+$	$4.00 \cdot 10^1$		[127]

Reversible aqueous-phase reactions implemented within the CAPRAM-HM3.0.

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	K	Ref.	$k_{f,298}$	E_A/R	Ref.	$k_{b,298}$	E_A/R	Ref.
E1②	$Cl + Cl^- \rightleftharpoons Cl_2^-$	$1.4 \cdot 10^5$		$8.50 \cdot 10^9$			$6.00 \cdot 10^4$		
E2②	$Cl_2 + Cl^- \rightleftharpoons Cl_3^-$	$1.80 \cdot 10^{-1}$		$2.00 \cdot 10^4$			$1.10 \cdot 10^5$		
E3②	$Cl_2 + H_2O \rightleftharpoons H^+ + Cl^- + HOCl$	$1.90 \cdot 10^{-5} e^{-4500/T}$		$4.00 \cdot 10^{-1}$	8000		$2.10 \cdot 10^4$	3500	
E4②	$HCl \rightleftharpoons H^+ + Cl^-$	$1.72 \cdot 10^6\ e^{6890/T}$		$5.00 \cdot 10^{11}$	-6890		$2.90 \cdot 10^5$		
E5②	$HOCl \rightleftharpoons H^+ + ClO^-$	$3.00 \cdot 10^{-8}$		$1.50 \cdot 10^3$			$5.00 \cdot 10^{10}$		
E6②	$Cl^- + OH \rightleftharpoons ClOH^-$	$7.00 \cdot 10^{-1}$		$4.30 \cdot 10^9$			$6.10 \cdot 10^9$		
E7②	$Cl + OH^- \rightleftharpoons ClOH^-$	$7.83 \cdot 10^8$		$1.80 \cdot 10^{10}$			$2.30 \cdot 10^1$		
E8②	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	$5.10 \cdot 10^6$		$2.10 \cdot 10^{10}$			$4.10 \cdot 10^3$		
E9②	$ClOH^- + Cl^- \rightleftharpoons Cl_2^- + OH^-$	$2.20 \cdot 10^{-4}$		$1.00 \cdot 10^4$			$4.50 \cdot 10^7$		
E10②	$Cl^- + SO_4^- \rightleftharpoons Cl + SO_4^{2-}$	$1.20 \cdot 10^0$		$2.52 \cdot 10^8$			$2.10 \cdot 10^8$		
E11②	$Cl^- + NO_3 \rightleftharpoons Cl + NO_3^-$	$3.40 \cdot 10^0\ e^{-4300/T}$		$3.40 \cdot 10^8$	4300		$1.00 \cdot 10^8$		
E12②	$Cl^- + Fe^{3+} \rightleftharpoons FeCl^{2+}$	$1.39 \cdot 10^0$		$3.00 \cdot 10^3$			$2.16 \cdot 10^3$		
E13	$HClO_2 \rightleftharpoons H^+ + ClO_2^-$	$1.91 \cdot 10^{-2}$	141	$9.55 \cdot 10^8$			$5.00 \cdot 10^{10}$		
E14	$ClO_2^- + O_3 \rightleftharpoons O_3^- + ClO_2$	$4.55 \cdot 10^1$		$8.19 \cdot 10^6$		142	$1.80 \cdot 10^5$		77
E15	$HOCl + NO_2^- \rightleftharpoons ClNO_2 + OH^-$	$3.97 \cdot 10^{-4}$	143	$1.99 \cdot 10^7$			$5.00 \cdot 10^{10}$		
E16	$Cl_2 + SO_4^{2-} \rightleftharpoons Cl^- + HOCl + HSO_4^-$	$1.14 \cdot 10^{-3}$		$3.20 \cdot 10^1$		144	$2.80 \cdot 10^3$		144
E17	$Cl_2 + HCOO^- \rightleftharpoons Cl^- + HOCl + HCOOH$	$1.00 \cdot 10^3$		$1.20 \cdot 10^2$		144	$1.20 \cdot 10^{-1}$		144
E18	$Cl_2 + CH_3COO^- \rightleftharpoons Cl^- + HOCl + CH_3COOH$	$3.36 \cdot 10^4$		$9.40 \cdot 10^2$		144	$2.80 \cdot 10^{-2}$		144
E19	$Cl_2 + CH_2ClCOO^- \rightleftharpoons Cl^- + HOCl + CH_2ClCOOH$	$3.34 \cdot 10^2$		$9.70 \cdot 10^1$		144	$2.90 \cdot 10^{-1}$		144
E20	$Cl_2^- + OH^- \rightleftharpoons Cl^- + ClOH^-$	$4.50 \cdot 10^3$		$4.50 \cdot 10^7$		145	$1.00 \cdot 10^4$		145
E21	$ClO_3^- + SO_4^- \rightleftharpoons ClO_3 + SO_4^{2-}$	$8.00 \cdot 10^0$		$4.00 \cdot 10^6$		146	$5.00 \cdot 10^5$		146
E22	$ClO_3^- + NO_3 \rightleftharpoons ClO_3 + NO_3^-$	$4.20 \cdot 10^0$		$3.49 \cdot 10^3$		146	$8.30 \cdot 10^2$		146
E23	$ClO^- + ClO_2 \rightleftharpoons ClO + ClO_2^-$	$2.53 \cdot 10^{-10} e^{-7337/T}$		$9.11 \cdot 10^{-1}$	7337	147	$3.60 \cdot 10^9$		147
E24	$Cl^- + ClO_3^- \rightleftharpoons Cl_2O_3^{2-}$	$5.00 \cdot 10^0$		$2.00 \cdot 10^0$		95	$4.00 \cdot 10^{-1}$		95
E25	$Cl_2O_3^{2-} + 2\ H^+ \rightleftharpoons Cl_2O_3H_2$	$9.09 \cdot 10^{-4}$		$2.00 \cdot 10^{-4}$		95	$2.20 \cdot 10^{-1}$		95
E26	$Cl_2O_3H_2 + H^+ \rightleftharpoons Cl_2O_2 + H^+$	$1.00 \cdot 10^{-1}$		$8.00 \cdot 10^2$		95	$8.00 \cdot 10^3$		95
E27⦸	$Cl^- + NO_2^+ \rightleftharpoons ClNO_2$	$1.44 \cdot 10^8$		$3.90 \cdot 10^{10}$		148	$2.70 \cdot 10^2$		148
E28②	$CH_2ClCO_3 + H_2O \rightleftharpoons CH_2ClC(OH)_2O_2$	$3.67 \cdot 10^2$		$1.10 \cdot 10^7$			$3.00 \cdot 10^4$		
E29②	$CH_2ClCOOH \rightleftharpoons CH_2ClCOO^- + H^+$	$1.75 \cdot 10^{-5}\ e^{46/T}$		$8.75 \cdot 10^5$	-46		$5.00 \cdot 10^{10}$		
E30②	$Br + Br^- \rightleftharpoons Br_2^-$	$6.32 \cdot 10^5$		$1.20 \cdot 10^{10}$			$1.90 \cdot 10^4$		

② already implemented in CAPRAM-HM2.1, ⦸ update of CAPRAM-HM2.1

	Reaction	K	Ref.	$k_{f,298}$	E_A/R	Ref.	$k_{b,298}$	E_A/R	Ref.
E31②	$Br_2 + Br^- \rightleftharpoons Br_3^-$	$1.75 \cdot 10^{1}$		$9.60 \cdot 10^{8}$			$5.50 \cdot 10^{7}$		
E32②	$Br_2 + H_2O \rightleftharpoons H^+ + Br^- + HOBr$	$1.06 \cdot 10^{-10} e^{-7500/T}$		$1.70 \cdot 10^{0}$	7500		$1.60 \cdot 10^{10}$		
E33②	$HBr \rightleftharpoons H^+ + Br^-$	$1.00 \cdot 10^{9}$		$5.00 \cdot 10^{11}$			$5.00 \cdot 10^{2}$		
E34②	$HOBr \rightleftharpoons H^+ + BrO^-$	$2.00 \cdot 10^{-9}$		$1.00 \cdot 10^{2}$			$5.00 \cdot 10^{10}$		
E35②	$Br^- + OH \rightleftharpoons BrOH^-$	$3.33 \cdot 10^{2}$		$1.10 \cdot 10^{10}$			$3.30 \cdot 10^{7}$		
E36②	$Br + OH^- \rightleftharpoons BrOH^-$	$3.10 \cdot 10^{3}$		$1.30 \cdot 10^{10}$			$4.20 \cdot 10^{6}$		
E37②	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	$1.80 \cdot 10^{12}$		$4.40 \cdot 10^{10}$			$2.45 \cdot 10^{-2}$		
E38②	$BrOH^- + Br^- \rightleftharpoons Br_2^- + OH^-$	$7.00 \cdot 10^{1}$		$1.90 \cdot 10^{8}$			$2.70 \cdot 10^{6}$		
E39②	$HOBr + HOBr \rightleftharpoons H^+ + Br^- + HBrO_2$	$6.70 \cdot 10^{-12}$		$2.00 \cdot 10^{-5}$			$3.00 \cdot 10^{6}$		
E40②	$HBrO_2 \rightleftharpoons H^+ + BrO_2^-$	$1.26 \cdot 10^{-5}$		$6.30 \cdot 10^{5}$			$5.00 \cdot 10^{10}$		
E41②	$HOBr + HBrO_2 \rightleftharpoons 2\ H^+ + Br^- + BrO_3^-$	$1.70 \cdot 10^{0}$		$3.20 \cdot 10^{0}$			$2.00 \cdot 10^{0}$		
E42②	$HBrO_2 + HBrO_2 \rightleftharpoons HOBr + H^+ + BrO_3^-$	$3.00 \cdot 10^{11}$		$3.00 \cdot 10^{3}$			$1.00 \cdot 10^{-8}$		
E43②	$Br_2O_4 + H_2O \rightleftharpoons H^+ + BrO_3^- + HBrO_2$	$5.26 \cdot 10^{1}$		$2.20 \cdot 10^{3}$			$4.20 \cdot 10^{1}$		
E44②	$Br_2O_4 \rightleftharpoons 2\ BrO_2$	$5.30 \cdot 10^{-5}$		$7.40 \cdot 10^{4}$			$1.40 \cdot 10^{9}$		
E45②	$Br^- + CO_3^- \rightleftharpoons Br + CO_3^{2-}$	$5.00 \cdot 10^{-2}$		$1.00 \cdot 10^{5}$			$2.00 \cdot 10^{6}$		
E46	$BrO_2^- + O_3 \rightleftharpoons O_3^- + BrO_2$	$1.78 \cdot 10^{-4}$		$8.90 \cdot 10^{4}$		142	$5.00 \cdot 10^{8}$		104
E47	$Br_2 + SO_4^{2-} + H_2O \rightleftharpoons HOBr + Br^- + HSO_4^-$	$6.15 \cdot 10^{-6}$		$2.28 \cdot 10^{4}$		149	$3.70 \cdot 10^{9}$		149
E48	$BrO^- + HCO_3^- \rightleftharpoons HOBr + CO_3^{2-}$	$1.30 \cdot 10^{-1}$		$3.90 \cdot 10^{7}$		107	$3.00 \cdot 10^{8}$		107
E49	$HOBr + NO_2^- \rightleftharpoons BrNO_2 + OH^-$	$9.86 \cdot 10^{-6}$	143	$4.93 \cdot 10^{5}$			$5.00 \cdot 10^{10}$		
E50②	$BrCl \rightleftharpoons HOBr + H^+ + Cl^- - H_2O$	$1.80 \cdot 10^{-5}$		$1.00 \cdot 10^{5}$			$5.60 \cdot 10^{9}$		
E51②	$BrCl^- \rightleftharpoons Br^- + Cl$	$1.60 \cdot 10^{-7}$		$1.90 \cdot 10^{3}$			$1.20 \cdot 10^{10}$		
E52②	$BrCl^- \rightleftharpoons Br + Cl^-$	$6.10 \cdot 10^{-4}$		$6.10 \cdot 10^{4}$			$1.00 \cdot 10^{8}$		
E53②	$BrCl^- + Br^- \rightleftharpoons Br_2^- + Cl^-$	$1.86 \cdot 10^{3}$		$8.00 \cdot 10^{9}$			$4.30 \cdot 10^{6}$		
E54②	$BrCl^- + Cl^- \rightleftharpoons Br^- + Cl_2^-$	$2.75 \cdot 10^{-8}$		$1.10 \cdot 10^{2}$			$4.00 \cdot 10^{9}$		
E55②	$Br_2Cl^- \rightleftharpoons BrCl + Br^-$	$5.60 \cdot 10^{-5}$		$4.30 \cdot 10^{5}$			$7.70 \cdot 10^{9}$		
E56②	$Br_2Cl^- \rightleftharpoons Br_2 + Cl^-$	$7.60 \cdot 10^{-1}$		$3.80 \cdot 10^{4}$			$5.00 \cdot 10^{4}$		
E57②	$BrCl_2^- \rightleftharpoons BrCl + Cl^-$	$1.70 \cdot 10^{-1}$		$1.70 \cdot 10^{5}$			$1.00 \cdot 10^{6}$		
E58②	$BrCl_2^- \rightleftharpoons Br^- + Cl_2$	$1.50 \cdot 10^{-6}$		$9.00 \cdot 10^{3}$			$6.00 \cdot 10^{9}$		
E59②	$Br^- + ClOH^- \rightleftharpoons BrCl^- + OH^-$	$3.33 \cdot 10^{2}$		$1.00 \cdot 10^{9}$			$3.00 \cdot 10^{6}$		
E60②	$BrOH^- + Cl^- \rightleftharpoons BrCl^- + OH^-$	$9.50 \cdot 10^{1}$		$1.90 \cdot 10^{8}$			$2.00 \cdot 10^{7}$		
E61	$BrO_2 + ClO_2^- \rightleftharpoons BrO_2^- + ClO_2$	$1.00 \cdot 10^{6}$		$3.60 \cdot 10^{7}$		80	$3.60 \cdot 10^{1}$		118
E62	$BrCl + BrCl \rightleftharpoons Cl_2 + Br_2$	$7.60 \cdot 10^{-3}$	150	$3.80 \cdot 10^{8}$			$5.00 \cdot 10^{10}$		

② already implemented in CAPRAM-HM2.1, ⃠ update of CAPRAM-HM2.1

	Reaction	K	Ref.	$k_{f,298}$	E_A/R	Ref.	$k_{b,298}$	E_A/R	Ref.
E63	$BrO^- + ClO_2 \rightleftharpoons BrO + ClO_2^-$	$1.28 \cdot 10^{-7} e^{-6615/T}$		$2.05 \cdot 10^{0}$	6615	147	$1.60 \cdot 10^{7}$		147
E64	$Br^- + ClO_3^- \rightleftharpoons BrOClO_2^{2-}$	$5.41 \cdot 10^{-4}$		$2.00 \cdot 10^{0}$		115	$3.70 \cdot 10^{3}$		115
E65	$BrOClO_2^{2-} + 2\ H^+ \rightleftharpoons BrOCl(OH)_2$	$4.00 \cdot 10^{-5}$		$1.00 \cdot 10^{-1}$		115	$2.50 \cdot 10^{3}$		115
E66	$Br_2 + ClO_2^- \rightleftharpoons ClO_2 + Br_2^-$	$1.18 \cdot 10^{-6}$		$1.30 \cdot 10^{3}$		116	$1.10 \cdot 10^{9}$		116
E67⃠	$Br^- + BrNO_2 \rightleftharpoons Br_2 + NO_2^-$	$2.60 \cdot 10^{0}$		$1.85 \cdot 10^{6}$		85	$7.11 \cdot 10^{5}$		85
E68②	$CH_2BrCO_3 + H_2O \rightleftharpoons CH_2BrC(OH)_2O_2$	$3.67 \cdot 10^{2}$		$1.10 \cdot 10^{7}$			$3.00 \cdot 10^{4}$		
E69②	$CH_2BrCOOH \rightleftharpoons CH_2BrCOO^- + H^+$	$1.75 \cdot 10^{-5}\ e^{46/T}$		$8.75 \cdot 10^{5}$	-46		$5.00 \cdot 10^{10}$		
E70②	$I + I^- \rightleftharpoons I_2^-$	$1.36 \cdot 10^{5}$		$9.10 \cdot 10^{9}$			$6.70 \cdot 10^{4}$		
E71②	$I_2 + I^- \rightleftharpoons I_3^-$	$7.13 \cdot 10^{2}$		$6.20 \cdot 10^{9}$			$8.70 \cdot 10^{6}$		
E72②	$HI \rightleftharpoons H^+ + I^-$	$3.20 \cdot 10^{9}$		$5.00 \cdot 10^{11}$			$1.56 \cdot 10^{2}$		
E73②	$HOI \rightleftharpoons H^+ + IO^-$	$3.16 \cdot 10^{-11}$		$1.58 \cdot 10^{0}$			$5.00 \cdot 10^{10}$		
E74②	$HOI + H^+ + I^- \rightleftharpoons I_2 + H_2O$	$1.47 \cdot 10^{12}$		$4.40 \cdot 10^{12}$			$3.00 \cdot 10^{0}$		
E75②	$HOI + HOI \rightleftharpoons HIO_2 + H^+ + I^-$	$1.25 \cdot 10^{-9}$		$2.50 \cdot 10^{1}$			$2.00 \cdot 10^{10}$		
E76②	$HOI + HOI \rightleftharpoons IO_2^- + 2\ H^+ + I^-$	$1.25 \cdot 10^{-9}$		$2.50 \cdot 10^{1}$			$2.00 \cdot 10^{10}$		
E77②	$HIO_2 \rightleftharpoons H^+ + IO_2^-$	$2.51 \cdot 10^{-2}$		$1.26 \cdot 10^{9}$			$5.00 \cdot 10^{10}$		
E78②	$HIO_3 \rightleftharpoons H^+ + IO_3^-$	$1.70 \cdot 10^{-1}$		$8.50 \cdot 10^{9}$			$5.00 \cdot 10^{10}$		
E79②	$HIO_2 + HOI \rightleftharpoons IO_3^- + I^- + 2\ H^+$	$2.00 \cdot 10^{-1}$		$2.40 \cdot 10^{2}$			$1.20 \cdot 10^{3}$		
E80②	$IO_2^- + HOI \rightleftharpoons IO_3^- + I^- + H^+$	$2.00 \cdot 10^{-1}$		$2.40 \cdot 10^{2}$			$1.20 \cdot 10^{3}$		
E81②	$IO_2^- + I_2 \rightleftharpoons IO_3^- + 2\ I^- + 2\ H^+ - H_2O$	$1.30 \cdot 10^{-13}$		$5.50 \cdot 10^{-5}$			$4.20 \cdot 10^{8}$		
E82	$I^- + Fe^{3+} \rightleftharpoons FeI^{2+}$	$1.00 \cdot 10^{-3}$		$6.30 \cdot 10^{-3}$		151	$6.30 \cdot 10^{0}$		152
E83	$HOI^- \rightleftharpoons I + OH^-$	$2.19 \cdot 10^{-1}$		$3.50 \cdot 10^{7}$		122	$1.60 \cdot 10^{8}$		122
E84	$I_2 + OH^- \rightleftharpoons I_2OH^-$	$5.00 \cdot 10^{0}$		$1.00 \cdot 10^{10}$		125	$2.00 \cdot 10^{9}$		125
E85	$I_2OH^- \rightleftharpoons HOI + I^-$	$8.30 \cdot 10^{0}$		$2.49 \cdot 10^{9}$		125	$3.00 \cdot 10^{8}$		125
E86②	$IBr + I^- \rightleftharpoons I_2 + Br^-$	$4.20 \cdot 10^{5}$		$2.00 \cdot 10^{9}$			$4.74 \cdot 10^{3}$		
E87②	$HOI + H^+ + Cl^- \rightleftharpoons ICl$	$1.20 \cdot 10^{4}$		$2.90 \cdot 10^{10}$			$2.40 \cdot 10^{6}$		
E88②	$HOI + H^+ + Br^- \rightleftharpoons IBr$	$5.10 \cdot 10^{6}$		$4.10 \cdot 10^{12}$			$8.00 \cdot 10^{5}$		
E89②	$ICl + Cl^- \rightleftharpoons ICl_2^-$	$7.70 \cdot 10^{1}$		$4.24 \cdot 10^{9}$			$5.50 \cdot 10^{7}$		
E90②	$IBr + Br^- \rightleftharpoons IBr_2^-$	$2.90 \cdot 10^{2}$		$4.93 \cdot 10^{6}$			$1.70 \cdot 10^{5}$		
E91②	$ICl + Br^- \rightleftharpoons IClBr^-$	$1.80 \cdot 10^{4}$		$7.70 \cdot 10^{9}$			$4.30 \cdot 10^{5}$		
E92②	$IBr + Cl^- \rightleftharpoons IClBr^-$	$1.30 \cdot 10^{0}$		$5.00 \cdot 10^{4}$			$3.80 \cdot 10^{4}$		
E93	$Br_2 + I_2 \rightleftharpoons IBr + IBr$	$1.30 \cdot 10^{5}$		$1.30 \cdot 10^{4}$		134	$1.00 \cdot 10^{-1}$		134
E94②	$CH_2ICO_3 + H_2O \rightleftharpoons CH_2IC(OH)_2O_2$	$3.67 \cdot 10^{2}$		$1.10 \cdot 10^{7}$			$3.00 \cdot 10^{4}$		

② already implemented in CAPRAM-HM2.1, ⃠ update of CAPRAM-HM2.1

	Reaction	K	Ref.	$k_{f,298}$	E_A/R	Ref.	$k_{b,298}$	E_A/R	Ref.
E95②	$CH_2ICOOH \rightleftharpoons CH_2ICOO^- + H^+$	$1.75 \cdot 10^{-5}\ e^{46/T}$		$8.75 \cdot 10^5$	-46		$5.00 \cdot 10^{10}$		

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