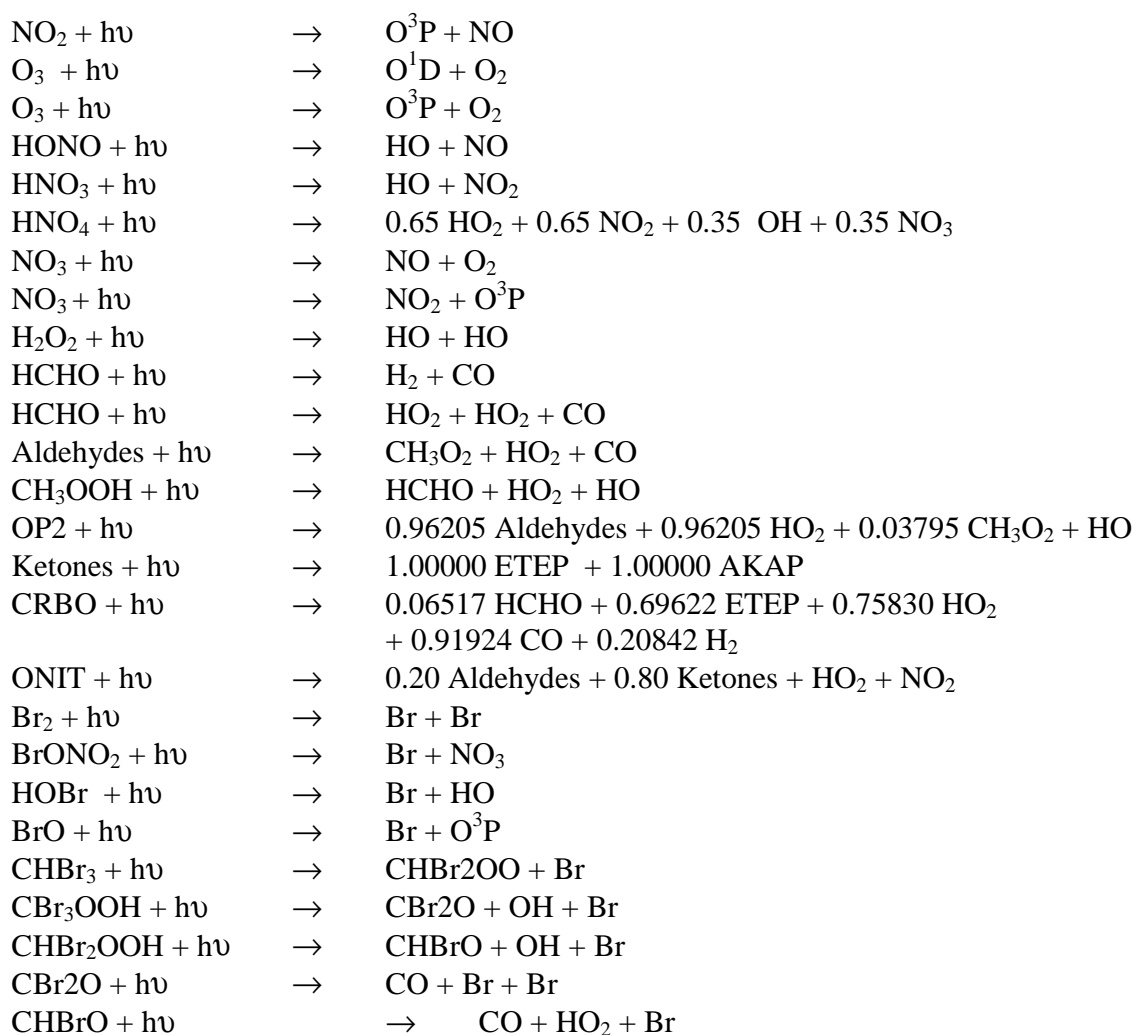


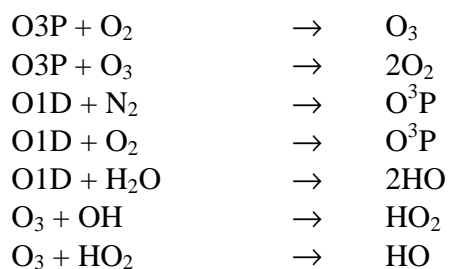
Chemical Reactions for the RELASH (RELACS + SHIVA) chemical mechanism

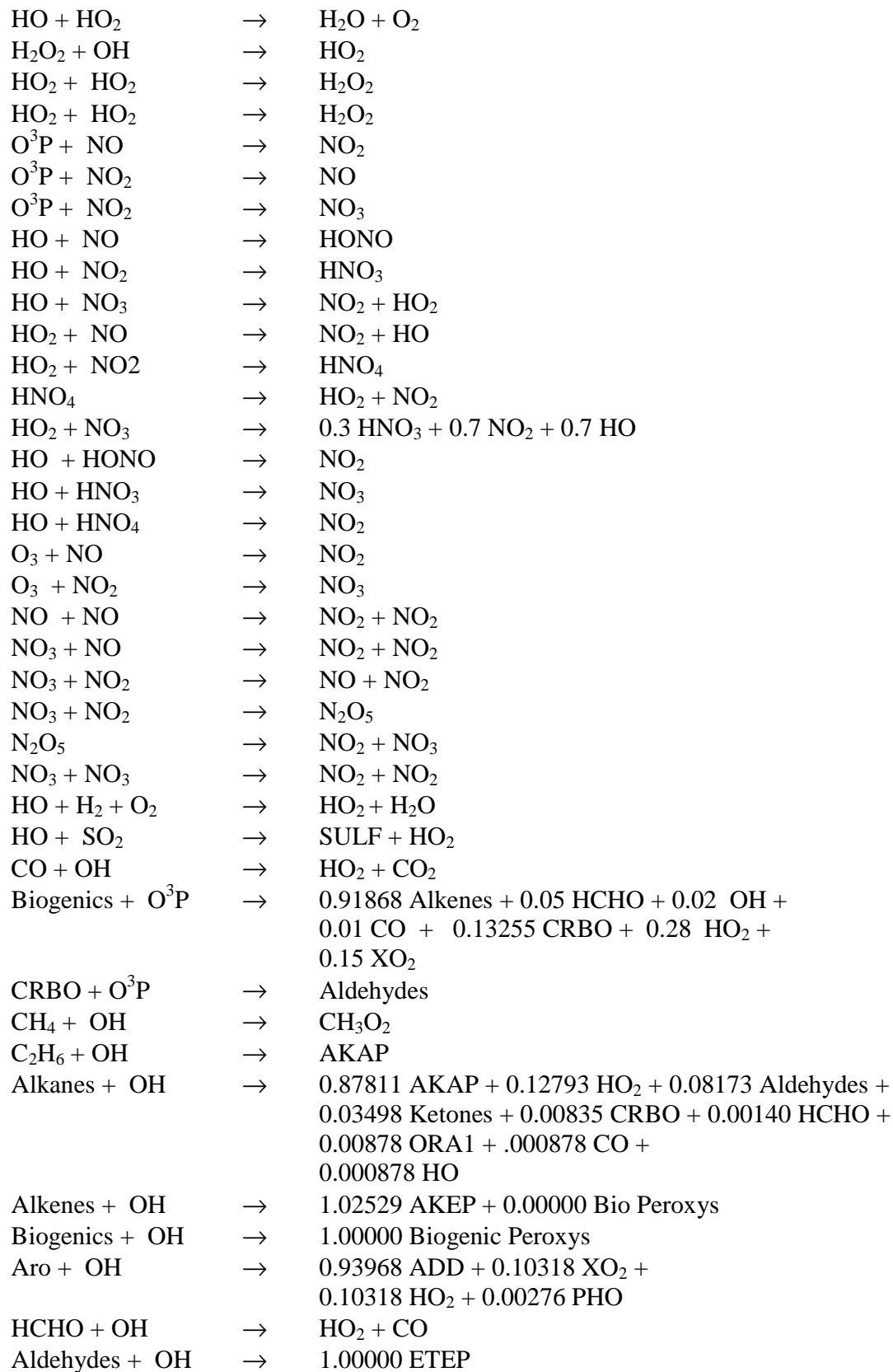
The RELACS component is based entirely off Crassier et al., 2000, and the halogen chemistry was added to C-CATT-BRAMS

Photolysis



Gas Phase

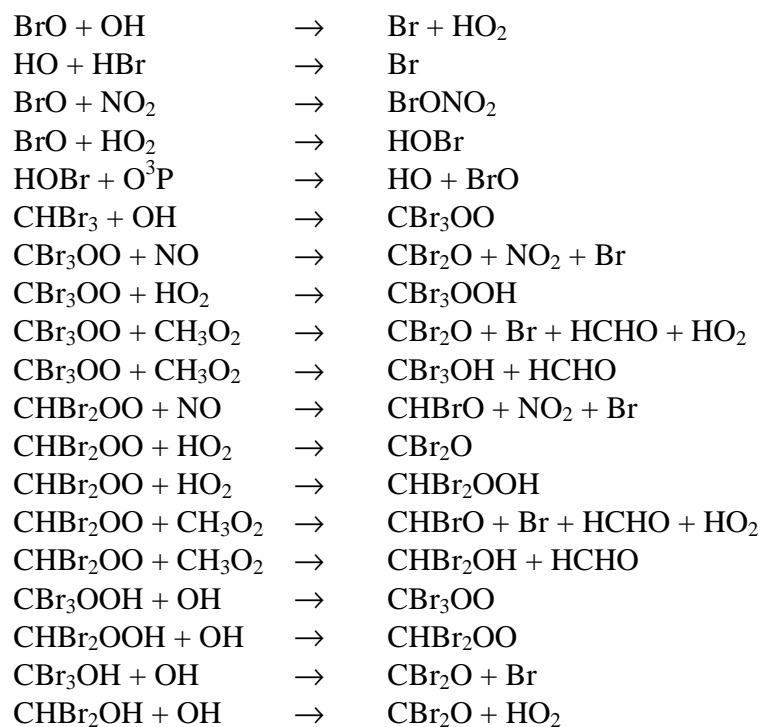




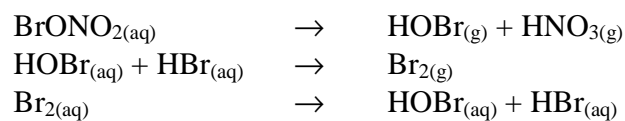
Ketones + OH	→	1.00000 ETEP
CRBO + OH	→	0.51419 ETEP + 0.16919 CRBO + 1.01732 CO + 0.51208 HO ₂ + 0.00000 HCHO + 0.06253 Aldehydes + 0.00853 Ketones + 0.10162 XO ₂ + 0.75196 H ₂ O
CH ₃ OOH + OH	→	0.65 CH ₃ O ₂ + 0.35 HCHO + 0.35 HO
OP2 + OH	→	0.40341 AKAP + 0.05413 ETEP + 0.07335 Aldehydes + 0.37591 Ketones + 0.09333 XO ₂ + 0.02915 HO ₂ + 0.02915 HCHO + 0.44925 HO
PAN + OH	→	0.57839 HCHO + 0.21863 CRBO + 0.71893 NO ₃ + 0.28107 PAN + 0.28107 HO ₂ + XO ₂ + 0.29733 H ₂ O
ONIT + OH	→	1.00000 AKAP + NO ₂
HCHO + NO ₃	→	HO ₂ + HNO ₃ + CO
Aldehydes + NO ₃	→	1.00000 ETEP + HNO ₃
CRBO + NO ₃	→	0.91567 HNO ₃ + 0.38881 ETEP + 0.10530 CRBO + 0.05265 Aldehydes + 0.00632 Ketones + 0.10530 NO ₂ + 0.10530 XO ₂ + 0.63217 HO ₂ + 1.33723 CO + 0.00000 OLN
Aro + NO ₃	→	HNO ₃ + PHO
Alkenes + NO ₃	→	0.00000 CRBO + 0.93768 OLN
Biogenics + NO ₃	→	0.91741 CRBO + 1.00000 OLN
PAN + NO ₃	→	0.60 ONIT + 0.60 NO ₃ + 0.40 PAN + 0.40 HCHO + 0.40 NO ₂ + XO ₂
Alkenes + O ₃	→	0.48290 HCHO + 0.51468 Aldehydes + 0.07377 Ketones + 0.00000 CRBO + 0.35120 CO + 0.15343 ORA1 + 0.08143 ORA2 + 0.23451 HO ₂ + 0.39435 OH + 0.05705 ETEP + 0.03196 C ₂ H ₆ + 0.00000 Alkenes + 0.04300 CH ₄ + 0.13966 CH ₃ O ₂ + 0.09815 AKAP + 0.01833 H ₂ O ₂ + 0.00000 XO ₂ + 0.05409 H ₂ + 0.00000 O ³ P
Biogenics + O ₃	→	0.90000 HCHO + 0.00000 Aldehydes + 0.00000 Ketones + 0.39754 CRBO + 0.36000 CO + 0.37388 Alkenes + 0.00000 AKAP + 0.17000 ETEP + 0.03000 CH ₃ O ₂ + 0.15000 ORA1 + 0.00000 ORA2 + 0.28000 OH + 0.30000 HO ₂ + 0.00100 H ₂ O ₂ + 0.05000 H ₂ + 0.13000 XO ₂ + 0.09000 O ³ P
CRBO + O ₃	→	0.00000 HCHO + 1.07583 CRBO + 0.15692 Aldehydes + 0.10788 ORA1 + 0.20595 ORA2 + 0.27460 ETEP + 0.10149 OP2 + 0.64728 CO + 0.28441 HO ₂ + 0.20595 OH + 0.00000 H ₂
PAN + O ₃	→	0.70 HCHO + 0.30 PAN + 0.70 NO ₂ + 0.13 CO + 0.04 H ₂ + 0.11 ORA1 + 0.08 HO ₂ + 0.036 OH + 0.70 ETEP
PHO + NO ₂	→	0.10670 Aro + ONIT

PHO + HO ₂	→	1.06698 Aro
ADD + NO ₂	→	Aro + HONO
ADD	→	0.98 Aro Peroxys + 0.02 Aro + 0.02 HO ₂
ADD + O ₃	→	Aro + HO
ETEP + NO ₂	→	1.00000 PAN
PAN	→	1.00000 ETEP + NO ₂
CH ₃ O ₂ + NO	→	HCHO + HO ₂ + NO ₂
AKAP + NO	→	0.33144 Aldehydes + 0.03002 HCHO + 0.54531 Ketones + 0.03407 CRBO + 0.74265 HO ₂ + 0.09016 CH ₃ O ₂ + 0.08187 AKAP + 0.13007 XO ₂ + 0.08459 ONIT + 0.91541 NO ₂
AKEP + NO	→	1.39870 HCHO + 0.42125 Aldehydes + 0.05220 Ketones + HO ₂ + NO ₂
Bio Peroxys+ NO	→	0.45463 CRBO + 0.60600 HCHO + 0.00000 Aldehydes + 0.00000 Ketones + 0.37815 Alkenes + 0.84700 HO ₂ + 0.84700 NO ₂ + 0.15300 ONIT
Aro Peroxys + NO	→	0.95115 NO ₂ + 0.95115 HO ₂ + 2.06993 CRBO + 0.04885 ONIT
ETEP + NO	→	0.78134 CH ₃ O ₂ + 0.09532 ETEP + 0.05848 HCHO + 0.07368 Aldehydes + 0.08670 CRBO + 0.12334 HO ₂ + 0.02563 XO ₂ + NO ₂
OLN + NO	→	0.18401 ONIT + 1.81599 NO ₂ + 0.18401 HO ₂ + 0.23419 HCHO + 1.01182 Aldehydes + 0.37862 Ketones
CH ₃ O ₂ + HO ₂	→	CH ₃ OOH
AKAP + HO ₂	→	1.00524 OP2
AKEP + HO ₂	→	1.00524 OP2
Bio Peroxys+ HO ₂	→	1.00524 OP2
Aro Peroxys + HO ₂	→	1.00524 OP2
ETEP + HO ₂	→	0.80904 OP2 + 0.17307 ORA2 + 0.17307 O ₃
OLN + HO ₂	→	ONIT
CH ₃ O ₂ + CH ₃ O ₂	→	1.33 HCHO + 0.66 HO ₂
AKAP + CH ₃ O ₂	→	0.80556 HCHO + 0.98383 HO ₂ + 0.56070 Aldehydes + 0.09673 Ketones + 0.01390 CH ₃ O ₂ + 0.07976 CRBO + 0.13370 XO ₂ + 0.00385 AKAP
AKEP + CH ₃ O ₂	→	1.42894 HCHO + 0.46413 Aldehydes + 0.03814 Ketones + HO ₂
Bio Peroxys + CH ₃ O ₂	→	0.56064 CRBO + 0.48074 Alkenes + 1.00000 HO ₂ + 1.09000 HCHO + 0.00000 Aldehydes + 0.00000 Ketones
Aro Peroxys + CH ₃ O ₂	→	HCHO + 1.02767 HO ₂ + 1.99461 CRBO
ETEP + CH ₃ O ₂	→	0.95723 HCHO + 0.82998 HO ₂ + 0.56031 CH ₃ O ₂ + 0.13684 ORA2 + 0.05954 ETEP + 0.15387 CRBO + 0.08295 Aldehydes + 0.02212 XO ₂
OLN + CH ₃ O ₂	→	0.88625 HCHO + 0.67560 HO ₂ + 0.67560 ONIT + 0.41524 Aldehydes + 0.09667 Ketones + 0.32440 NO ₂
AKAP + ETEP	→	0.71461 Aldehydes + 0.48079 HO ₂ + 0.51480 CH ₃ O ₂ + 0.49810 ORA2 + 0.18819 Ketones + 0.07600 HCHO +

		0.00828 AKAP + 0.11306 XO ₂ + 0.06954 CRBO
AKEP + ETEP	→	0.68192 HCHO + 0.68374 Aldehydes + 0.50078 HO ₂ + 0.50078 CH ₃ O ₂ + 0.49922 ORA2 + 0.06579 Ketones
Bio Peroxys+ ETEP	→	0.78591 CRBO + 0.24463 Alkenes + 0.50600 HO ₂ + 0.49400 ORA2 + 0.34000 HCHO + 0.50600 CH ₃ O ₂ + 0.00000 Aldehydes + 0.00000 Ketones
Aro Peroxys + ETEP	→	CH ₃ O ₂ + HO ₂ + 1.99455 CRBO
ETEP + ETEP	→	1.66702 CH ₃ O ₂ + 0.05821 ETEP + 0.03432 HCHO + 0.10777 CRBO + 0.06969 Aldehydes + 0.02190 Ketones + 0.07566 HO ₂ + 0.01593 XO ₂ + 0.09955 ORA2
OLN + ETEP	→	0.66562 ONIT + 0.51037 CH ₃ O ₂ + 0.48963 ORA2 + 0.17599 HO ₂ + 0.13414 HCHO + 0.42122 Aldehydes + 0.10822 Ketones + 0.00000 NO ₂
OLN + OLN	→	2.00 ONIT + HO ₂
OLN + OLN	→	.353 HCHO + .925 Aldehydes + .217 Ketones + 0.500 HO ₂ + .750 NO ₂ + 1.250 ONIT
CH ₃ O ₂ + NO ₃	→	HCHO + HO ₂ + NO ₂
AKAP + NO ₃	→	0.33743 Aldehydes + 0.81290 HO ₂ + 0.03142 HCHO + 0.62978 Ketones + 0.03531 CRBO + 0.09731 CH ₃ O ₂ + 0.08994 AKAP + 0.16271 XO ₂ + NO ₂
AKEP + NO ₃	→	1.40909 HCHO + 0.43039 Aldehydes + 0.02051 Ketones + HO ₂ + NO ₂
Bio Peroxys + NO ₃	→	0.61160 CRBO + 0.42729 Alkenes + 0.68600 HCHO + 0.00000 Aldehydes + 0.00000 Ketones + HO ₂ + NO ₂
Aro Peroxys + NO ₃	→	2.81904 CRBO + HO ₂ + NO ₂
ETEP + NO ₃	→	0.91910 CH ₃ O ₂ + 0.03175 ETEP + 0.03175 HCHO + 0.03455 CRBO + 0.02936 Aldehydes + 0.04915 HO ₂ + 0.01021 XO ₂ + NO ₂
OLN + NO ₃	→	0.25928 ONIT + 1.74072 NO ₂ + 0.25928 HO ₂ + 0.20740 HCHO + 0.91850 Aldehydes + 0.34740 Ketones
XO ₂ + HO ₂	→	1.00524 OP2
XO ₂ + CH ₃ O ₂	→	HCHO + HO ₂
XO ₂ + ETEP	→	CH ₃ O ₂
XO ₂ + XO ₂	→	
XO ₂ + NO	→	NO ₂
XO ₂ + NO ₃	→	NO ₂
HCHO + Br	→	HO ₂ + CO + HBr
Br + O ₃	→	BrO
BrO + O3P	→	Br
BrO + NO	→	NO ₂ + Br
BrO + BrO	→	Br + Br
Br + HO ₂	→	HBr
O ¹ D + HBr	→	HO + Br



Aqueous Phase



OP2 = C₂ and higher organic peroxides

ORA2 = C₂ and higher organic acids

ONIT = Organic nitrate

ETEP = Peroxy radicals from ethane

XO₂ = Species accounting for additional NO to NO₂ conversions