Methanol-derived HO_2 radical reactions

Reaction	Rate Coefficient / $molecule^{-1}cm^3s^{-1}$
$HO_2 + NO \rightarrow OH$	8.6×10^{-12}

Methane-derived HO_2 radical reactions

Reaction	Rate Coefficient / $molecule^{-1}cm^3s^{-1}$
$CH_3O_2 + NO \rightarrow CH_3O$	7.7×10^{-12}
$CH_3O_2 + NO \rightarrow$ Loss	7.7×10^{-15}
$CH_3O + O_2 \rightarrow HO_2$	1.9×10^{-15}
$CH_3O + NO \rightarrow$ Loss	1.7×10^{-11}
$HO_2 + NO \rightarrow OH$	8.6×10^{-12}

Propane-derived RO_2 radical reactions[1]

Reaction	Rate Coefficient / $molecule^{-1}cm^3s^{-1}$
$i\text{-}C_3H_7O_2 + NO \rightarrow i\text{-}C_3H_7O$	8.7×10^{-12}
$n\text{-}C_3H_7O_2 + NO \rightarrow n\text{-}C_3H_7O$	9.2×10^{-12}
$i\text{-}C_3H_7O_2 + NO \rightarrow$ Loss	3.8×10^{-13}
$n\text{-}C_3H_7O_2 + NO \rightarrow$ Loss	1.9×10^{-13}
$i\text{-}C_3H_7O + O_2 \rightarrow HO_2$	6.9×10^{-15}
$n\text{-}C_3H_7O + O_2 \rightarrow HO_2$	1.1×10^{-14}
$i\text{-}C_3H_7O + NO \rightarrow$ Loss	3.3×10^{-11}
$n\text{-}C_3H_7O + NO \rightarrow$ Loss	3.3×10^{-11}
$HO_2 + NO \rightarrow OH$	8.6×10^{-12}

[1] Ratio of [$n\text{-}C_3H_7O_2$] and [$i\text{-}C_3H_7O_2$] determined from branching ratio of the reaction RH + OH in MCMv3.2,

n-Butane-derived RO_2 radical reactions[1]

Reaction	Rate Coefficient / $molecule^{-1}cm^3s^{-1}$
$n\text{-}C_4H_9O_2 + NO \rightarrow n\text{-}C_4H_9O$	8.7×10^{-12}
$n\text{-}C_4H_9O_2 + NO \rightarrow$ Loss	3.0×10^{-13}
$n\text{-}C_4H_9O + O_2 \rightarrow HO_2$	1.4×10^{-14}
$n\text{-}C_4H_9O + O_2 \rightarrow (HO)C_4H_8O_2$	1.9×10^{5} †
$n\text{-}C_4H_9O + NO \rightarrow$ Loss	3.3×10^{-11}
$(HO)C_4H_8O_2 + NO \rightarrow (HO)C_4H_8O$	8.9×10^{-12}
$(HO)C_4H_8O_2 + NO \rightarrow$ Loss	1.2×10^{-13}
$(HO)C_4H_8O \rightarrow HO_2$	8.8×10^{6}
$i\text{-}C_4H_9O_2 + NO \rightarrow i\text{-}C_4H_9O$	8.2×10^{-12}
$i\text{-}C_4H_9O_2 + NO \rightarrow$ Loss	8.1×10^{-13}
$i\text{-}C_4H_9O + O_2 \rightarrow HO_2$	7.7×10^{-15}
$i\text{-}C_4H_9O + NO \rightarrow$ Loss	3.3×10^{-11}
$i\text{-}C_4H_9O \rightarrow C_2H_5O_2$	4.6×10^{5} †
$C_2H_5O_2 + NO \rightarrow C_2H_5O$	9.1×10^{-12}
$C_2H_5O_2 + NO \rightarrow$ Loss	8.2×10^{-14}
$C_2H_5O + O_2 \rightarrow HO_2$	8.1×10^{-15}
$C_2H_5O + NO \rightarrow$ Loss	3.3×10^{-11}

HO_2 + NO → OH	8.6×10^{-12}

[1] Ratio of [n-$C_4H_9O_2$] and [i-$C_4H_9O_2$] determined from branching ratio of the reaction RH + OH in MCMv3.2, † Rate coefficient for isomerisation at 298 K

Cyclohexane-derived RO_2 radical reactions[1]

Reaction	Rate Coefficient / molecule^{-1}cm^{3}s^{-1}
CHEXO2 + NO → CHEXO	8.3×10^{-12}
CHEXO2 + NO → Loss	7.1×10^{-13}
CHEXO + O_2 → CO1C6O2*	6.3×10^{4} †
CHEXO + O_2 → HO_2	9.1×10^{-15}
CHEXO + NO → Loss	3.3×10^{-11}
CO1C6O2 + NO → CO1C6O*	8.3×10^{-12}
CO1C6O2 + NO → Loss*	7.1×10^{-13}
CO1C6O → CO1H63O2*	1.0×10^{6}
CO1C6O + NO → Loss*	3.3×10^{-11}
CO1H63O2 + NO → CO1H63O*	8.3×10^{-12}
CO1H63O2 + NO → Loss*	7.1×10^{-13}
CO1H63O → HO_2*	1.0×10^{6}
CO1H63O + NO → Loss*	3.3×10^{-11}
HO_2 + NO → OH*	8.6×10^{-12}

* Reactions assuming ring-opening occurs, † Rate coefficient for ring opening at 298 K

n-Pentane-derived RO_2 radical reactions[1]

Reaction	Rate Coefficient / molecule^{-1}cm^{3}s^{-1}
PECO2 + NO → PECO	7.5×10^{-12}
PECO2 + NO → Loss	1.1×10^{-12}
PECO + O_2 → HO_2	7.3×10^{-15}
PECO + O_2 → $C_2H_5O_2$	2.6×10^{4} †
PECO + NO → Loss	3.3×10^{-11}
$C_2H_5O_2$ + NO → C_2H_5O	9.1×10^{-12}
$C_2H_5O_2$ + NO → Loss	8.2×10^{-14}
C_2H_5O + O_2 → HO_2	8.1×10^{-15}
PEBO2 + NO → PEBO	7.5×10^{-12}
PEBO2 + NO → Loss	1.1×10^{-12}
PEBO + O_2 → HO2C5O2	1.8×10^{5} †
PEBO + O_2 → HO_2	9.1×10^{-15}
PEBO + NO → Loss	3.3×10^{-11}
HO2C5O2 + NO → HO2C5O	8.4×10^{-12}
HO2C5O2 + NO → Loss	1.8×10^{-13}
HO2C5O → HO_2	2.0×10^{7}
HO2C5O + NO → Loss	3.3×10^{-11}
PEAO2 + NO → PEAO	8.2×10^{-12}
PEAO2 + NO → Loss	4.5×10^{-13}
PEAO + O_2 → HO1C5O2	1.8×10^{6} †
PEAO + NO → Loss	3.3×10^{-11}
HO1C5O2 + NO → HO1C5O	8.2×10^{-12}

HO1C5O2 + NO → Loss	4.5×10^{-13}
HO1C5O → HO_2	7.8×10^{6}
HO1C5O + NO → Loss	3.3×10^{-11}
HO_2 + NO → OH	8.6×10^{-12}

[1]Ratio of [PEAO2], [PEBO2] and [PECO2] determined from branching ratio of the reaction RH + OH in MCMv3.2 , [†] Rate coefficient for isomerisation at 298 K

Isoprene-derived RO_2 radical reactions[1]

Reaction	Rate Coefficient / $molecule^{-1}cm^{3}s^{-1}$
ISOPAO2 + NO → ISOPAO	7.7×10^{-12}
ISOPAO2 + NO → Loss	8.6×10^{-13}
ISOPAO → HO_2	2.5×10^{5}
ISOPAO → C524O2	7.5×10^{5}
ISOPAO + NO → Loss	3.3×10^{-11}
C524O2 + NO → C524O	7.5×10^{-12}
C524O2 + NO → Loss	1.2×10^{-12}
C524O → HO_2	1.0×10^{6}
C524O + NO → Loss	3.3×10^{-11}
ISOPBO2 + NO → ISOPBO	8.0×10^{-12}
ISOPBO2 + NO → Loss	5.7×10^{-13}
ISOPBO → HO_2	1.0×10^{6}
ISOPBO + NO → Loss	3.3×10^{-11}
ISOPCO2 + NO → ISOPCO	7.7×10^{-12}
ISOPCO2 + NO → Loss	8.6×10^{-13}
ISOPCO → HO_2	1.0×10^{6}
ISOPCO + NO → Loss	3.3×10^{-11}
ISOPDO2 + NO → ISOPDO	7.5×10^{-12}
ISOPDO2 + NO → Loss	1.2×10^{-12}
ISOPDO → HO_2	1.0×10^{6}
ISOPDO + NO → Loss	3.3×10^{-11}
HO_2 + NO → OH	8.6×10^{-12}

[1]Ratio of [ISOPAO2], [ISOPBO2], [ISOPCO2] and [ISOPDO2] determined from branching ratio of the reaction RH + OH in MCMv3.2

Ethene-derived RO_2 radical reactions

Reaction	Rate Coefficient / $molecule^{-1}cm^{3}s^{-1}$
$HOCH_2CH_2O_2$ + NO → $HOCH_2CH_2O$	9.0×10^{-12}
$HOCH_2CH_2O_2$ + NO → Loss	4.5×10^{-14}
$HOCH_2CH_2O$ + O_2 → HO_2	9.1×10^{-15}
$HOCH_2CH_2O$ → HCHO + CH_2OH	5.1×10^{5} [†]
$HOCH_2CH_2O$ + NO → Loss	3.3×10^{-11}
CH_2OH + O_2 → HO_2	1.0×10^{-11}
HO_2 + NO → OH	8.6×10^{-12}

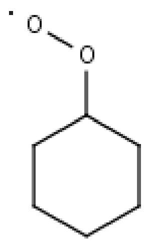
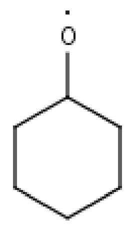
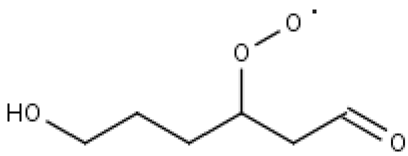
[†] Rate coefficient for decomposition at 298 K

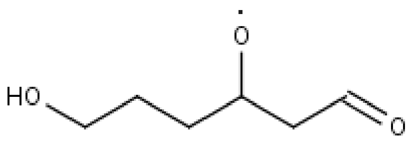
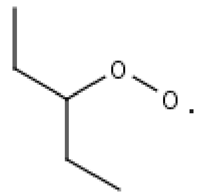
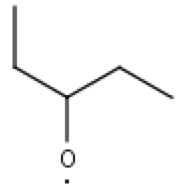
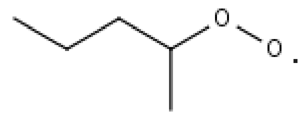
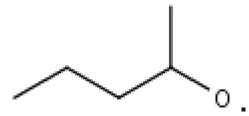
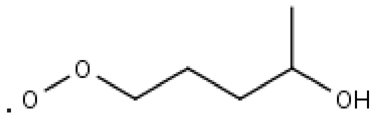
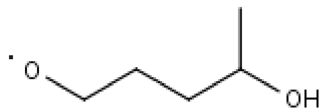
Toluene-derived RO_2 radical reactions[1]

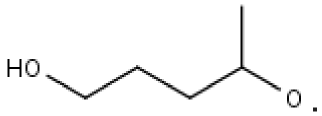
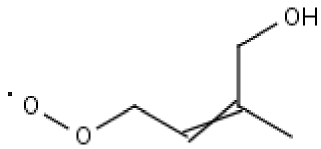
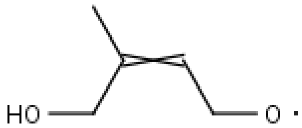
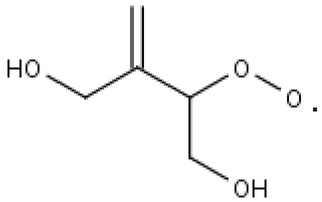
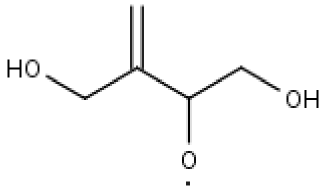
Reaction	Rate Coefficient / $molecule^{-1}cm^{3}s^{-1}$

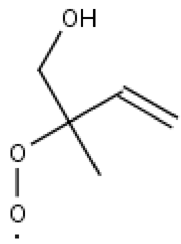
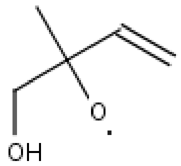
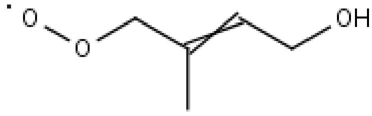
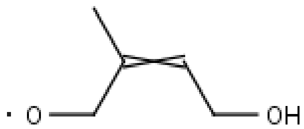
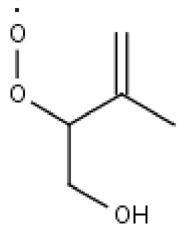
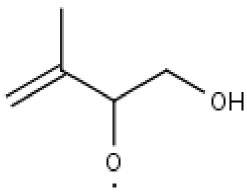
$C_6H_5CH_2O_2$ + NO → $C_6H_5CH_2O$	8.1×10^{-12}
$C_6H_5CH_2O_2$ + NO → Loss	9.5×10^{-13}
$C_6H_5CH_2O$ + O_2 → HO_2	9.1×10^{-15}
$C_6H_5CH_2O$ + NO → Loss	3.3×10^{-11}
$TLBIPERO_2$ + NO → TLBIPERO	8.0×10^{-12}
$TLBIPERO_2$ + NO → Loss	1.0×10^{-12}
TLBIPERO → HO_2	1.0×10^{6}
TLBIPERO + NO → Loss	3.3×10^{-11}
HO_2 + NO → OH	8.6×10^{-12}

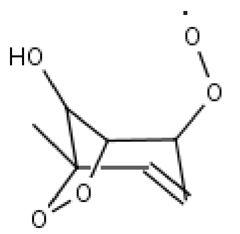
[1]Ratio of [$C_6H_5CH_2O_2$], [HO_2] and [$TLBIPERO_2$] determined from branching ratio of the reaction RH + OH in MCMv3.2

MCM species name	Structural formula
CHEXO2	
CHEXO	
CO1C6O2	
CO1C6O	
CO1H63O2	

CO1H63O	
PECO2	
PECO	
PEBO2	
PEBO	
HO2C5O2	
HO2C5O	
PEAO2	

PEAO	
HO1C5O2	
HO1C5O	
ISOPAO2	
ISOPAO	
C524O2	
C524O	

ISOPBO2	
ISOPBO	
ISOPCO2	
ISOPCO	
ISOPDO2	
ISOPDO	

TLBIPERO$_2$	
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