

SAPRC07T Mechanism Species

Species	Definition	Molecular weight
ACETONE	Acetone	58.08
ACETYLENE	Acetylene	26.04
ACROLEIN	Acrolein	56.06
ACROLEIN_PRIMARY	Acrolein emissions tracer	56.06
AFG1	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form radicals	98.10
AFG2	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form non-radical products	98.10
AFG3	Lumped diunsaturated dicarbonyl aromatic fragmentation product.	124.14
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2×10^2 and 5×10^2 ppm ⁻¹ min ⁻¹ . (Primarily ethane)	30.07
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5×10^2 and 2.5×10^3 ppm ⁻¹ min ⁻¹ . (Primarily propane and acetylene)	36.73
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5×10^3 and 5×10^3 ppm ⁻¹ min ⁻¹ .	58.61
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5×10^3 and 1×10^4 ppm ⁻¹ min ⁻¹ .	77.6
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than 1×10^4 ppm ⁻¹ min ⁻¹ .	118.89

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Species	Definition	Molecular weight
ALK5RXN	SOA precursor compounds products from largest alkanes (ALK5)	118.9
APIN	α -pinene	136.23
ARO1	Aromatics with kOH < 2×10^4 ppm ⁻¹ min ⁻¹ .	95.16
ARO2	Aromatics with kOH > 2×10^4 ppm ⁻¹ min ⁻¹ .	118.72
BACL	Biacetyl	86.09
BALD	Aromatic aldehydes (e.g., benzaldehyde)	106.13
BENZENE	Benzene	78.11
BNZHRXN	SOA precursor compounds from benzene via peroxy radical reaction with HO ₂	127
BNZNRXN	SOA precursor compounds from benzene via peroxy radical reaction with NO	127
BNZRO2	SOA precursor surrogate from benzene	127
BUTADIENE13	1,3-butadiene	54.09
BZCO3	Peroxyacyl radical formed from Aromatic Aldehydes	137.11
BZO	Phenoxy Radicals	93
CCHO	Acetaldehyde	44.05
CCHO_PRIMARY	Acetaldehyde Emissions Tracer	44.05
CCOOH	Acetic Acid. Also used for peroxyacetic acid in Carter	60.05
CCOOOH	Proposed for Peroxyacetic Acid	76
CH4	Methane, held constant	16.04
CL	Chlorine atoms	35.5
CL2	Chlorine molecules	70
CLACET	Chloroacetone (and other alpha-chloro ketones that are assumed to be similarly photoreactive)	92.5
CLCCHO	Chloroacetaldehyde (and other alpha-chloro aldehydes that are assumed to be similarly photoreactive)	78.5
CLCHO	Formyl Chloride (assumed to be unreactive)	64.5
CLNO	Nitrosyl Chloride	65.5
CLNO2	Nitryl Chloride	83.5

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CLO	ClO. Radicals	51.5
CLONO	ClONO	81.5
CLONO2	ClONO2	96.5
CO	Carbon Monoxide	28.01
CO2	Carbon Dioxide	44.01
COOH	Methyl Hydroperoxide	48.04
CRES	Phenols and Cresols	108.14
ETHENE	Ethene	28.05
ETOH	Ethanol	46.068
GLY	Glyoxal	58.04
H2	Hydrogen Molecules	2.016
H2O	Water	18.02
HCHO	Formaldehyde	30.03
HCHO_PRIMARY	Formaldehyde Emission Tracer	30.03
HCL	Hydrochloric acid	36.5
HCOOH	Formic Acid	46.03
HNO3	Nitric Acid	63.02
HNO4	Peroxynitric Acid	79.02
HO2	Hydroperoxide Radicals	33.01
HO2H	Hydrogen Peroxide	34.01
HOCCHO	Glycolaldehyde	60.05
HOCL	HOCl	52.5
HOCOO	Radical formed when Formaldehyde reacts with HO2	51
HONO	Nitrous Acid	47.02
HV	Light	0
IPRD	Lumped isoprene product species	100.12
ISOPRENE	Isoprene	68.12
ISOPRXN	SOA precursor compounds from isoprene	68
M	Air	28.85
MACO3	Peroxyacyl radicals formed from methacrolein and other acroleins.	101.08
MACR	Methacrolein	70.09
MAPAN	PAN analogue formed from Methacrolein	147.09

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MECO3	Acetyl Peroxy Radicals	75.04
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5×10^{-13} but slower than 5×10^{-12} cm ³ molec ⁻² sec ⁻¹ . (Based on mechanism for methyl ethyl ketone).	72.11
MEO2	Methyl Peroxy Radicals	47.03
MEOH	Methanol	32.04
MGLY	Methyl Glyoxal	72.07
MVK	Methyl Vinyl Ketone	70.09
MXYL	m-xylene	106.16
N2O5	Nitrogen Pentoxide	108.02
NO	Nitric Oxide	30.01
NO2	Nitrogen Dioxide	46.01
NO2EX	Electronically excited NO ₂ (only needed if reaction with H ₂ O forming OH is non-negligible)	44
NO3	Nitrate Radical	62.01
NPHE	Nitrophenols	139.11
O1D	Excited Oxygen Atoms	16
O2	Oxygen	31.99
O3	Ozone	47.99
O3P	Ground State Oxygen Atoms	16
OH	Hydroxyl Radicals	17.01
OLE1	Alkenes (other than ethene) with $k_{OH} < 7 \times 10^4$ ppm ⁻¹ min ⁻¹ .	72.34
OLE2	Alkenes with $k_{OH} > 7 \times 10^4$ ppm ⁻¹ min ⁻¹ .	75.78
OXYL	o-xylene	106.16
PAN	Peroxy Acetyl Nitrate	121.05
PAN2	PPN and other higher alkyl PAN analogues	135.08
PBZN	PAN analogues formed from Aromatic Aldehydes	183.13

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Species	Definition	Molecular weight
PRD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than $5 \times 10^{-12} \text{ cm}^3 \text{ molec}^{-2} \text{ sec}^{-1}$.	116.16
PROPENE	propene	42.08
PXYL	p-xylene	106.16
R6OOH	Lumped organic hydroperoxides with 5 or more carbons (other than those formed following OH addition to aromatic rings, which is represented separately). Mechanism based on that estimated for 3-hexyl hydroperoxide.	118.17
RAOOH	Organic hydroperoxides formed following OH addition to aromatic rings, which is represented separately because of their probable role in SOA formation. Mechanism based on two isomers expected to be formed in the m-xylene system.	188.18
RCHO	Lumped C3+ Aldehydes (mechanism based on propionaldehyde)	58.08
RCO3	Peroxy Propionyl and higher peroxy acyl Radicals	89.07
RCOOH	Higher organic acids and, in Carter, peroxy acids (mechanism based on propionic acid).	74.08
RCOOOH	Proposed Higher organic peroxy acids	74.08
RNO3	Lumped Organic Nitrates	147.18
RO2C	Peroxy Radical Operator representing NO to NO2 and NO3 to NO2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals.	1

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Species	Definition	Molecular weight
RO2XC	Peroxy Radical Operator representing NO consumption (used in conjunction with organic nitrate formation), and the effects of peroxy radical reactions on NO ₃ , acyl peroxy radicals, and other peroxy radicals.	1
ROOH	Lumped organic hydroperoxides with 2-4 carbons. Mechanism based on that estimated for n-propyl hydroperoxide.	76.1
SESQ	Sesquiterpenes	204.35
SESQRXN	SOA precursor compounds from sesquiterpenes	204
SO2	Sulfur Dioxide	64.06
SULF	Sulfates (SO ₃ or H ₂ SO ₄)	98.08
SULRXN	Sulfate Aerosol Percusor	98.08
TBUO	t-Butoxy Radicals	73
TERP	Terpenes	136.24
TOLHRXN	SOA precursor compounds from toluene and less reactive aromatics (ARO1) via peroxy radical reaction with HO ₂	147.60
TOLNRXN	SOA precursor compounds from toluene and less rective aromatics (ARO1) via peroxy radical reaction with NO	147.60
TOLRO2	SOA precursor surrogate from toluene and ARO1 reactions with OH	147.6
TOLUENE	toluene	92.14
TRIMETH_BENZ124	1,2,4-trimethyl benzene	120.19
TRPRXN	SOA precursor compounds from α -pinene and terpenes	136
xACETONE	As above, but for ACETONE	58.08
xACROLEIN	As above, but for ACROLEIN	56.06
xAFG1	As above, but for AFG1	98.1
xAFG2	As above, but for AFG2	98.1
xAFG3	As above, but for AFG3	124.74
xBACL	As above, but for BACL	86.09
xBALD	As above, but for BALD	106.13

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Species	Definition	Molecular weight
xCCHO	As above, but for CCHO	44.05
xCL	Formation of Cl radicals from alkoxy radicals formed in peroxy radical reactions with NO and NO ₃ (100% yields) and RO ₂ (50% yields)	35.5
xCLACET	As above, but for CLACET	92.5
xCLCCHO	As above, but for CLCCHO	78.5
xCO	As above, but for CO	28.01
xGLY	As above, but for GLY	58.04
xHCHO	As above, but for HCHO	30.03
xHO ₂	Formation of HO ₂ from alkoxy radicals formed in peroxy radical reactions with NO and NO ₃ (100% yields) and RO ₂ (50% yields)	33.01
xHOCCHO	As above, but for HOCCHO	60.05
xIPRD	As above, but for IPRD	100.12
xMACO ₃	As above, but for MACO ₃	101.08
xMACR	As above, but for MACR	70.09
xMECO ₃	As above, but for MECO ₃	75.04
xMEK	As above, but for MEK	72.11
xMEO ₂	As above, but for MEO ₂	47.03
xMGLY	As above, but for MGLY	72.07
xMVK	As above, but for MVK	70.09
xNO ₂	As above, but for NO ₂	46.01
xOH	As above, but for OH	17.01
xPROD ₂	As above, but for PROD ₂	116.16
xRCHO	As above, but for RCHO	58.08
xRCO ₃	As above, but for RCO ₃	89.07
xRNO ₃	As above, but for RNO ₃	147.18
xTBUO	As above, but for TBUO	73
XYLHRXN	SOA precursor compounds from xylene and higher reactive aromatics (ARO ₂) via peroxy radical reaction with HO ₂	167.70

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Species	Definition	Molecular weight
XYLNRXN	SOA precursor compounds from xylene and higher reactive aromatics (ARO2) via peroxy radical reaction with NO	167.70
XYLRO2	SOA precursor surrogate from xylene and ARO2 reactions with OH	167.20
yR6OOH	As above, but the RO2 + HO2 product is represented by R6OOH and the H-shift products are represented by PROD2.	118.17
yRAOOH	As above, but for RAOOH	188.18
yROOH	Formation of ROOH following RO2 + HO2 reactions, or formation of H-shift disproportionation products (represented by MEK) in the RO2 + RCO3 and (in 50% yields) RO2 + RO2 reactions.	76.1
zRNO3	Formation of RNO3 in the RO2 + NO, reaction, or formation of corresponding non-nitrate products (represented by PROD2) formed from alkoxy radicals formed in RO2 + NO3 and (in 50% yields) RO2 + RO2 reactions.	147.18