

**Species in MOZART-T1 with Stratosphere, Mesosphere and Lower Thermosphere
(CESM2 TSLMT/WACCM mechanism)**

Species	Chemical Formula	Description
ACBZO2	C ₇ H ₅ O ₃	acylperoxy radical from benzaldehyde
ALKNIT	C ₅ H ₁₁ ONO ₂	standard alkyl nitrate from BIGALK+OH chemistry
ALKO2	C ₅ H ₁₁ O ₂	lumped alkane peroxy radical from BIGALK
ALKOOH	C ₅ H ₁₂ O ₂	lumped alkane hydroperoxide
APIN	C ₁₀ H ₁₆	alpha-pinene
AOA_NH	CO	age of air tracer
BCARY	C ₁₅ H ₂₄	beta-caryophyllene and other sesquiterpenes
BENZENE	C ₆ H ₆	benzene
BENZO2	C ₆ H ₇ O ₅	bicyclic peroxy radical from OH + benzene
BENZOOH	C ₆ H ₈ O ₅	bicyclic hydroperoxide from OH + benzene
BEPOMUC	C ₆ H ₆ O ₃	unsaturated dialdehydic epoxide from OH + benzene
BIGALD1	C ₄ H ₄ O ₂	butenedial, a product of aromatic oxidation
BIGALD2	C ₅ H ₆ O ₂	4-oxo-2-pentenal, a product of aromatic oxidation
BIGALD3	C ₅ H ₆ O ₂	2-methyl butenedial, a product of aromatic oxidation
BIGALD4	C ₆ H ₈ O ₂	2-methyl-4-oxo-2-pentenal, a product of aromatic oxidation
BIGALD	C ₅ H ₆ O ₂	lumped aldehyde from terpene ozonolysis
BIGALK	C ₅ H ₁₂	lumped alkanes C>3
BIGENE	C ₄ H ₈	lumped alkenes C>3
BPIN	C ₁₀ H ₁₆	beta-pinene
BR	Br	bromine atom
BRCL	BrCl	bromine chloride
BRO	BrO	bromine monoxide
BRONO2	BrONO ₂	bromine nitrate
BRY	Br _y	total reactive bromine
BZALD	C ₇ H ₆ O	benzaldehyde
BZOO	C ₇ H ₇ O ₂	peroxy radical from toluene oxidation
BZOOH	C ₇ H ₈ O ₂	hydroperoxide from toluene oxidation
C2H2	C ₂ H ₂	ethyne (acetylene)
C2H4	C ₂ H ₄	ethene
C2H5O2	C ₂ H ₅ O ₂	ethylperoxy radical
C2H5OH	C ₂ H ₅ OH	ethanol
C2H5OOH	C ₂ H ₅ OOH	ethyl hydroperoxide
C2H6	C ₂ H ₆	ethane
C3H6	C ₃ H ₆	propene
C3H7O2	C ₃ H ₇ O ₂	propylperoxy radical
C3H7OOH	C ₃ H ₇ OOH	propyl hydroperoxide
C3H8	C ₃ H ₈	propane
C6H5O2	C ₆ H ₅ O ₂	phenylperoxy radical
C6H5OOH	C ₆ H ₅ OOH	phenyl hydroperoxide
CCL4	CCl ₄	carbon tetrachloride
CF2CLBR	CF ₂ ClBr	bromochlorodifluoromethane (Halon 1211)

CF3Br	CF ₃ Br	bromotrifluoromethane (Halon 1301)
CFC113	CCl ₂ FCClF ₂	1,1,2-trichlorotrifluoroethane
CFC114	CClF ₂ CClF ₂	1,2-dichloro-tetrafluoroethane
CFC115	CClF ₂ CF ₃	chloropentafluoroethane
CFC11	CFCl ₃	trichlorofluoromethane
CFC12	CF ₂ Cl ₂	dichlorodifluoromethane
CH2BR2	CH ₂ Br ₂	dibromomethane (methylene bromide)
CH2O	CH ₂ O	formaldehyde
CH3BR	CH ₃ Br	methyl bromide
CH3CCL3	CH ₃ CCl ₃	mehtylchloroform
CH3CHO	CH ₃ CHO	acetaldehyde
CH3CL	CH ₃ Cl	methyl chloride
CH3CN	CH ₃ CN	acetonitrile
CH3CO3	CH ₃ CO ₃	acetylperoxy radical
CH3COCH3	CH ₃ COCH ₃	acetone
CH3COCHO	CH ₃ COCHO	methyl glyoxal
CH3COOH	CH ₃ COOH	acetic acid
CH3COOOH	CH ₃ COOOH	peracetic acid
CH3O2	CH ₃ O ₂	methylperoxy radical
CH3OH	CH ₃ OH	methanol
CH3OOH	CH ₃ OOH	methyl hydroperoxide
CH4	CH ₄	methane
CHBr3	CHBr ₃	bromoform
CL2	Cl ₂	chlorine
CL2O2	Cl ₂ O ₂	chlorine monoxide dimer
CL	Cl	chlorine atom
CLO	CIO	chlorine monoxide
CLONO2	CIONO ₂	chlorine nitrate
CLY	Cl _y	total reactive chlorine
CO2	CO ₂	carbon dioxide
CO	CO	carbon monoxide
COF2	COF ₂	carbonyl fluoride
COFCL	COFCl	carbonyl chlorofluoride
CRESOL	C ₇ H ₈ O	lumped cresols (hydroxymethylbenzenes)
DICARBO2	C ₅ H ₅ O ₄	acylperoxy radical formed from aromatic oxidation, via unsaturated dicarbonyl chemistry
DMS	CH ₃ SCH ₃	dimethyl sulfide
E90	CO	artificial tracer with 90-day lifetime
ENEO2	C ₄ H ₉ O ₃	lumped hydroxyperoxy radical from OH + large alkenes
EO2	HOCH ₂ CH ₂ O ₂	hydroxyperoxy radical from OH + ethene chemistry
EO	HOCH ₂ CH ₂ O	hydroxalkoxy radical from OH + ethene chemistry
EOOH	HOCH ₂ CH ₂ OOH	hydroxyhydroperoxide from OH + ethene chemistry
F	F	fluorine atom
GLYALD	HOCH ₂ CHO	glycolaldehyde
GLYOXAL	C ₂ H ₂ O ₂	glyoxal
H2402	CBrF ₂ CBrF ₂	dibromotetrafluoroethane (Halon 2402)

H2	H ₂	hydrogen
H2O2	H ₂ O ₂	hydrogen peroxide
H2SO4	H ₂ SO ₄	sulfuric acid
H	H	hydrogen atom
HBr	HBr	hydrogen bromide
HCFC141B	CH ₃ CCl ₂ F	1,1-dichoro-1-fluoroethane
HCFC142B	CH ₃ CClF ₂	1-chloro-1,1-difluoroethane
HCFC22	CHF ₂ Cl	chlorodifluoromethane
HCL	HCl	hydrogen chloride
HCN	HCN	hydrogen cyanide
HCOOH	HCOOH	formic acid
HF	HF	hydrogen fluoride
HMPROP	C ₄ H ₈ O ₂	hydroxymethylpropanal, OH+MBO product
HMPROPO2	C ₄ H ₇ O ₄	peroxy radical from HMPROP oxidation
HNO3	HNO ₃	nitric acid
HO2	HO ₂	hydroperoxyl radical
HO2NO2	HO ₂ NO ₂	pernitric acid
HOBr	HOBr	hypobromous acid
HOCH2OO	HOCH ₂ OO	formaldehyde / HO ₂ adduct
HOCL	HOCl	hypochlorous acid
HONITR	C ₄ H ₉ NO ₄	lumped hydroxynitrates from various compounds
HPALD	C ₅ H ₈ O ₃	unsaturated hydroperoxyaldehyde, from isoprene chemistry
HYAC	CH ₃ COCH ₂ OH	hydroxyacetone
HYDRALD	C ₅ H ₈ O ₂	lumped unsaturated hydroxycarbonyl
IEPOX	C ₅ H ₁₀ O ₃	isoprene-derived epoxide
ISOP	C ₅ H ₈	isoprene
ISOPAO2	HOC ₅ H ₈ O ₂	1,2-isomer of isoprene peroxy radical
ISOPBO2	HOC ₅ H ₈ O ₂	1,4-isomer of isoprene peroxy radical
ISOPNITA	C ₅ H ₉ NO ₄	1,2-hydroxynitrate from OH+isoprene chemistry
ISOPNITB	C ₅ H ₉ NO ₄	1,4-hydroxynitrate from OH+isoprene chemistry
ISOPNO3	C ₅ H ₈ NO ₅	peroxy radical from isoprene NO ₃ oxidation
ISOPNOOH	C ₅ H ₉ NO ₅	nitrooxy-hydroperoxide from NO ₃ +isoprene chemistry
ISOPOOH	C ₅ H ₁₀ O ₃	unsaturated hydroxyhydroperoxide
IVOC	C ₁₃ H ₂₈	intermediate volatility organic precursor of VBS SOA
LIMON	C ₁₀ H ₁₆	limonene
MACR	CH ₂ CCH ₃ CHO	methacrolein
MACRO2	C ₄ H ₇ O ₃	peroxy radical from OH addition to methacrolein
MACROOH	C ₄ H ₈ O ₄	peroxide from methacrolein
MALO2	C ₄ H ₃ O ₄	acylperoxy radical from OH reaction with BIGALD1
MBO	C ₅ H ₁₀ O	2-methyl-3-buten-2-ol
MBONO3O2	C ₅ H ₁₀ NO ₆	peroxy radical from NO ₃ +MBO
MBOO2	C ₅ H ₁₁ O ₄	peroxy radical from OH+MBO
MBOOOH	C ₅ H ₁₂ O ₄	hydroperoxide from OH+MBO
MCO3	CH ₂ CCH ₃ CO ₃	peroxy radical from OH abstraction reaction with MACR
MDIALO2	C ₄ H ₅ O ₄	peroxy radical from OH addition to BIGALD1
MEK	C ₄ H ₈ O	methyl ethyl ketone

MEKO2	C ₄ H ₇ O ₃	peroxy radical formed from MEK oxidation
MEKO OH	C ₄ H ₈ O ₃	hydroperoxide from MEK oxidation
MPAN	CH ₂ CCH ₃ CO ₃ NO ₂	methacryloyl peroxy nitrate
MTERP	C ₁₀ H ₁₆	lumped monoterpenes
MVK	CH ₂ CHCOCH ₃	methyl vinyl ketone
MYRC	C ₁₀ H ₁₆	limonene
N2D	N	electronically excited nitrogen atoms
N2O5	N ₂ O ₅	dinitrogen pentoxide
N2O	N ₂ O	nitrous oxide
N2p	N ₂	N2+
N	N	nitrogen atom
NC4CH2OH	C ₅ H ₉ NO ₄	nitrooxy-alcohol from NO3+isoprene chemistry
NC4CHO	C ₅ H ₇ NO ₄	nitrooxy-aldehyde from NO3+isoprene chemistry
NDEP	N	diagnostic of nitrogen deposition
NH3	NH ₃	ammonia
NH4	NH ₄	ammonium ion aerosol
NHDEP	N	diagnostic of ammonia deposition
NH_50	CO	idealized tracer with 50-day loss rate
NH_5	CO	idealized tracer with 5-day loss rate
NO2	NO ₂	nitrogen dioxide
NO3	NO ₃	nitrate radical
NO	NO	nitric oxide
NOA	CH ₃ COCH ₂ ONO ₂	nitrooxyacetone, largely from NO3+propene chemistry
NOp	NO	NO+
NTERPO2	C ₁₀ H ₁₆ NO ₅	peroxy radical from NO3+terpene chemistry
NTERPOOH	C ₁₀ H ₁₇ NO ₅	nitrooxy-hydroperoxide from NO3+terpene chemistry
Np	N	N ⁺
O1D	O	excited state atomic oxygen
O2	O ₂	oxygen
O2_1D	O ₂	first excited state of O ₂ (Delta)
O2_1S	O ₂	second excited state of O ₂ (Sigma)
O2p	O ₂	O ₂ ⁺
O3	O ₃	ozone
O3S	O ₃	stratospheric ozone tracer
O	O	ground state atomic oxygen
OCLO	OCIO	chlorine dioxide
OCS	OCS	carbonyl sulfide
OH	OH	hydroxyl radical
ONITR	C ₄ H ₇ NO ₄	lumped hydroxynitrates (formula updated 2017-04-06)
Op	O	Op
PAN	CH ₃ CO ₃ NO ₂	peroxy acetyl nitrate
PBZNIT	C ₇ H ₅ O ₃ NO ₂	peroxy benzoyl nitrate
PHENO2	C ₆ H ₇ O ₆	bicyclic peroxy radical from phenol
PHENO	C ₆ H ₅ O	phenoxy radical
PHENOL	C ₆ H ₅ OH	phenol, product of benzene chemistry
PHENOOH	C ₆ H ₈ O ₆	bicyclic hydroperoxide from phenol

PO2	C ₃ H ₆ OHO ₂	propene-derived peroxy radical
POOH	C ₃ H ₆ OHO ₂	propene-derived hydroxy hydroperoxide
RO2	CH ₃ COCH ₂ O ₂	peroxy radical from acetone
ROOH	CH ₃ COCH ₂ OOH	acetone hydroperoxide
S	S	atomic sulfur
SF6	SF ₆	sulfur hexafluoride
SO2	SO ₂	sulfur dioxide
SO3	SO ₃	sulfur trioxide
SO	SO	sulfur monoxide
SOAG0	C ₁₅ H ₃₈ O ₂	SOA gas-phase precursor VBS bin 0 (mol.wt. = 250 g/mol [Shrivastava et al., JGR, 2015])
SOAG1	C ₁₅ H ₃₈ O ₂	SOA gas-phase precursor VBS bin 1
SOAG2	C ₁₅ H ₃₈ O ₂	SOA gas-phase precursor VBS bin 2
SOAG3	C ₁₅ H ₃₈ O ₂	SOA gas-phase precursor VBS bin 3
SOAG4	C ₁₅ H ₃₈ O ₂	SOA gas-phase precursor VBS bin 4
ST80_25	CO	Stratospheric loss tracer
SVOC	C ₂₂ H ₄₆	semi-volatile organic precursor of VBS SOA
TEPOMUC	C ₇ H ₈ O ₃	toluene, xylenes product
TERP2O2	C ₁₀ H ₁₅ O ₄	peroxy radical from lumped terpene product oxidation
TERP2OOH	C ₁₀ H ₁₈ O ₃	hydroxy hydroperoxide from terpene 2 double bonds
TERPNIT	C ₁₀ H ₁₇ NO ₄	mostly hydroxynitrates from OH+terpene chemistry
TERPO2	C ₁₀ H ₁₇ O ₃	peroxy radical from terpenes+OH
TERPOOH	C ₁₀ H ₁₈ O ₃	hydroxy hydroperoxide from terpene 0 double bonds
TERPROD1	C ₁₀ H ₁₆ O ₂	lumped terpene oxidation product
TERPROD2	C ₉ H ₁₄ O ₂	lumped terpene oxidation product (2 nd generation)
TOLO2	C ₇ H ₉ O ₅	bicyclic peroxy radical from toluene
TOLOOH	C ₇ H ₁₀ O ₅	bicyclic hydroperoxide from toluene
TOLUENE	C ₇ H ₈	toluene
XO2	C ₅ H ₉ O ₅	peroxy radical from ISOPOOH, IEPOX, HPALD
XOOH	C ₅ H ₁₀ O ₅	lumped hydroperoxide from XO2 chemistry
XYLENES	C ₈ H ₁₀	lumped xylenes
XYLENO2	C ₈ H ₁₁ O ₅	bicyclic peroxy radical from OH+xylenes chemistry
XYLENOOH	C ₈ H ₁₂ O ₅	bicyclic hydroperoxide from OH+xylenes chemistry
XYLOL	C ₈ H ₁₀ O	dimethyl phenol from xylenes oxidation
XYLOLO2	C ₈ H ₁₁ O ₆	bicyclic peroxy radical from OH+XYLOL chemistry
XYLOLOOH	C ₈ H ₁₂ O ₆	bicyclic hydroperoxide from OH+XYLOL chemistry

Aerosols

NH4	NH ₄	ammonium bulk aerosol
bc_a1	C	black carbon, MAM accumulation mode
bc_a4	C	black carbon, MAM primary carbon mode
dst_a1	AlSiO ₅	dust, MAM accumulation mode
dst_a2	AlSiO ₅	dust, MAM Aitken mode
dst_a3	AlSiO ₅	dust, MAM coarse mode
ncl_a1	NaCl	sea salt, MAM accumulation mode
ncl_a2	NaCl	sea salt, MAM Aitken mode

ncl_a3	NaCl	sea salt, MAM coarse mode
num_a1	H	aerosol number concentration, MAM accumulation mode
num_a2	H	aerosol number concentration, MAM Aitken mode
num_a3	H	aerosol number concentration, MAM coarse mode
num_a4	H	aerosol number concentration, MAM primary carbon mode
pom_a1	C	primary organic matter, MAM accumulation mode
pom_a4	C	primary organic matter, MAM primary carbon mode
so4_a1	NH ₄ HSO ₄	sulfate aerosol, MAM accumulation mode
so4_a2	NH ₄ HSO ₄	sulfate aerosol, MAM Aitken mode
so4_a3	NH ₄ HSO ₄	sulfate aerosol, MAM coarse mode
soa1_a1	C ₁₅ H ₃₈ O ₂	SOA bin 1, MAM accumulation mode
soa1_a2	C ₁₅ H ₃₈ O ₂	SOA bin 1, MAM Aitken mode
soa2_a1	C ₁₅ H ₃₈ O ₂	SOA bin 2, MAM accumulation mode
soa2_a2	C ₁₅ H ₃₈ O ₂	SOA bin 2, MAM Aitken mode
soa3_a1	C ₁₅ H ₃₈ O ₂	SOA bin 3, MAM accumulation mode
soa3_a2	C ₁₅ H ₃₈ O ₂	SOA bin 3, MAM Aitken mode
soa4_a1	C ₁₅ H ₃₈ O ₂	SOA bin 4, MAM accumulation mode
soa4_a2	C ₁₅ H ₃₈ O ₂	SOA bin 4, MAM Aitken mode
soa5_a1	C ₁₅ H ₃₈ O ₂	SOA bin 5, MAM accumulation mode
soa5_a2	C ₁₅ H ₃₈ O ₂	SOA bin 5, MAM Aitken mode

Species with dry deposition:

ALKNIT, ALKOOH, BENZOOH, BZOOH, C2H5OH, C2H5OOH, C3H7OOH, C6H5OOH, CH2O, CH3CHO, CH3CN, CH3COCH₃, CH3COCCHO, CH3COOH, CH3COOOH, CH3OH, CH3OOH, CO, EOOH, GLYALD, H₂O₂, H₂SO₄, HCN, HCOOH, HNO₃, HO₂NO₂, HONITR, HPALD, HYAC, HYDRALD, IEPOX, ISOPNITA, ISOPNITB, ISOPNO₃, ISOPNOOH, ISOPOOH, IVOC, MACROOH, MEKO OH, MPAN, NC4CH2OH, NC4CHO, NH₃, NH₄, NO, NO₂, NOA, NTERPOOH, O₃, ONITR, PAN, PHENOOH, POOH, ROOH, SO₂, SOAG0, SOAG1, SOAG2, SOAG3, SOAG4, SVOC, TERP2OOH, TERPNIT, TERPOOH, TERPROD1, TERPROD2, TOLOOH, XOOH, XYLENOOH, XYLOLOOH, bc_a1, bc_a4, dst_a1, dst_a2, dst_a3, ncl_a1, ncl_a2, ncl_a3, num_a1, num_a2, num_a3, num_a4, pom_a1, pom_a4, so4_a1, so4_a2, so4_a3, soa1_a1, soa1_a2, soa2_a1, soa2_a2, soa3_a1, soa3_a2, soa4_a1, soa4_a2, soa5_a1, soa5_a2

Species with wet deposition:

ALKNIT, ALKOOH, BENZOOH, BRONO₂, BZOOH, C2H5OH, C2H5OOH, C3H7OOH, C6H5OOH, CH2O, CH3CHO, CH3CN, CH3COCH₃, CH3COCCHO, CH3COOH, CH3COOOH, CH3OH, CH3OOH, CLONO₂, COF₂, COFCL, EOOH, GLYALD, H₂O₂, H₂SO₄, HBR, HCL, HCN, HCOOH, HF, HNO₃, HO₂NO₂, HOBr, HOCl, HONITR, HPALD, HYAC, HYDRALD, IEPOX, ISOPNITA, ISOPNITB, ISOPNO₃, ISOPNOOH, ISOPOOH, IVOC, MACR, MACROOH, MEKO OH, MVK, NC4CH2OH, NC4CHO, NDEP, NH₃, NH₄, NHDEP, NOA, NTERPOOH, ONITR, PHENOOH, POOH, ROOH, SO₂, SOAG0, SOAG1, SOAG2, SOAG3, SOAG4, SVOC, TERP2OOH, TERPNIT, TERPOOH, TERPROD1, TERPROD2, TOLOOH, XOOH, XYLENOOH, XYLOLOOH,

bc_a1, bc_a4, dst_a1, dst_a2, dst_a3, ncl_a1, ncl_a2, ncl_a3, num_a1, num_a2, num_a3,
num_a4, pom_a1, pom_a4, so4_a1, so4_a2, so4_a3, soa1_a1, soa1_a2, soa2_a1, soa2_a2,
soa3_a1, soa3_a2, soa4_a1, soa4_a2, soa5_a1, soa5_a2