Appendix A – CMAQ Chemical Mechanisms and Species

Table A-2. CB05tucl species

Species	Description	MW
AACD	Acetic and higher acids	60
ALD2	Acetaldehyde	44
ALDX	Propionaldehyde and higher aldehydes	44
BENZENE	Benzene	78
BENZRO2	First generation SOA intermediate from benzene oxidation	127
BNZHRXN	Counter species for computing SOA from BENZENE under low NOx conditions	127
BNZNRXN	Counter species for computing SOA from BENZENE under high NOx conditions	127
C2O3	Acetylperoxy radical	75
CAO2		133
CAT1		124
CL		35.5
CL2		71
CLO		51.5

CO	Carbon monoxide	28
CRES	Cresol and higher molecular weight phenols	108
CRN2		168
CRNO	Alkoxy radical from oxidation of CRON	152
CRO	Methylphenoxy radical	107
CRON	Nitro cresol	153
CRPX		169
CXO3	C3 and higher acylperoxy radicals	75
ETH	Ethene	28
ETHA	Ethane	30
ETOH	Ethanol	46
FACD	Formic acid	46
FMCL		64.5
FORM	Formaldehyde	30
H2O2	Hydrogen peroxide	34
HCL		36.5
HCO3		63
HNO3	Nitric acid	63
HO2	Hydroperoxy radical	33
HOCL		52.5
HONO	Nitrous acid	47
IOLE	Internal olefin carbon bond (R-C=C-R)	48
ISOP	Isoprene	68
ISOPRXN	Counter species for computing SOA from ISOP	68

ISPD	Isoprene oxidation product	70
MEO2	Methylperoxy radical	47
MEOH	Methanol	32
MEPX	Methylhydroperoxide	48
MGLY	Methylglyoxal and other aromatic products	72
N2O5	Nitrogen pentoxide	108
NO	Nitric oxide	30
NO2	Nitrogen dioxide	46
NO3	Nitrogen trioxide	62
NTR	Organic nitrate	130
O	Oxygen atom (triplet)	16
O1D	Oxygen atom (singlet)	16
O3	Ozone	48
OH	Hydroxyl radical	17
OLE	Terminal olefin carbon bond (R-C=C)	27
OPAN		161
OPEN	Aromatic ring open product	84
OPO3	Peroxyacyl radical from oxidation of OPEN	115
PACD	Peroxy acetic acid	76
PAN	Peroxyacyl nitrate	121
PANX	C3 and higher peroxyacyl nitrates	121
PAR	Paraffin carbon bond (C-C)	14
PNA	Peroxynitric acid	79
ROOH	Higher organic peroxide	62

ROR	Secondary alkoxy radical	31
SESQ	Sesquiterpene	204
SESQRXN	Counter species for computing SOA from SESQ	204
SO2	Sulfur dioxide	64
SULF	Sulfuric acid gas	98
SULRXN	Counter species for computing aerosols from SULF	98
TERP	Terpene	136
TO2	Tolene-hydroxyl radical adduct	173
TOL	Toluene and other monoalkyl aromatics	92
TOLHRXN	Counter species for computing SOA from TOL under low NOx conditions	141
TOLNRXN	Counter species for computing SOA from TOL under high NOx conditions	141
TOLRO2	First generation SOA intermediate from TOL oxidation	141
TRPRXN	Counter species for computing SOA from TERP	136
XO2	NO-to-NO2 conversion from alkylperoxy radical	1
XO2N	NO-to-nitrate conversion from alkylperoxy radical	1
XYL	Xylene and other polyalkyl aromatics	106
XYLHRXN	Counter species for computing SOA from XYL under low NOx conditions	155
XYLNRXN	Counter species for computing SOA from XYL under high NOx conditions	155

XYLRO2	First generation SOA intermediate from XYL oxidation	155

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