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{created automatically by xmecca, DO NOT EDIT!}
{xmecca was run on 2024-11-30 at 15:26:02 by matthias on machine matthias-Z390-I-AORUS-
PRO-WIFI}
{***** START: gas-phase species from gas.spc *****}
{Time-stamp: <2019-01-09 16:19:59 sander>}
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{-----}
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{ SYNTAX AND NAMING CONVENTIONS FOR KPP SPECIES }
{ - Species are sorted by elements in the following order: }
{   O,H,N,C,F,Cl,Br,I,S,Hg }
{ - Organics are sorted by increasing number of C, H, O, N }
{ - All peroxides are called R00H, all peroxy radicals are called R02 }
{ - All species are defined here with #DEFVAR as VARIABLES. Some species }
{   will be turned into FIXED species with #SETFIX in messy_mecca_kpp.kpp }
{ - Lumped species start with the letter "L". }
{ - The maximum length for the species name is 13 (15 may also be ok?). }
{ - The species name must not contain the underscore character "_". }
{ - The elemental composition is needed for graphviz (spc_extract.awk) and }
{   to check the mass balance (check_conservation.pl). There must be spaces }
{   around the "+" sign but no spaces between a number and the element }
{   symbol. }
{ - The name of the species in LaTeX syntax follows after the "@" sign. }
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{-----}
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#DEFVAR
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{-----}
{----- gas phase -----}
{-----}
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{----- O -----}
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01D	= 0	; {@O(^1D)}	{0 singlet D}
03P	= 0	; {@O(^3P)}	{0 triplet P}
O2	= 2O	; {@O_2}	{oxygen}
O3	= 3O	; {@O_3}	{ozone}

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{----- H -----}
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H	= H	; {@H}	{hydrogen atom}
H2	= 2H	; {@H_2}	{hydrogen}
OH	= H + O	; {@OH}	{hydroxyl radical}
HO2	= H + 2O	; {@HO_2}	{hydroperoxy radical}
H2O	= 2H + O	; {@H_2O}	{water}
H2O2	= 2H + 2O	; {@H_2O_2}	{hydrogen peroxide}
H2OH2O	= 4H + 2O	; {@(H_2O)_2}	{water dimer}

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{----- N -----}
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N	= N	; {@N}	{nitrogen atom}
N2D	= N	; {@N(^2D)}	{N doublet D}
N2	= 2N	; {@N_2}	{nitrogen}
NH3	= 3H + N	; {@NH_3}	{ammonia}
N2O	= O + 2N	; {@N_2O}	{nitrous oxide}
NO	= O + N	; {@NO}	{nitric oxide}
NO2	= 2O + N	; {@NO_2}	{nitrogen dioxide}
NO3	= 3O + N	; {@NO_3}	{nitrogen trioxide}
N2O5	= 5O + 2N	; {@N_2O_5}	{dinitrogen pentoxide}
HONO	= H + 2O + N	; {@HONO}	{nitrous acid}
HN03	= H + 3O + N	; {@HNO_3}	{nitric acid}
HN04	= H + 4O + N	; {@HNO_4}	{peroxynitric acid}
NH2	= 2H + N	; {@NH_2}	{}
HNO	= H + O + N	; {@HNO}	{}
NHOH	= 2H + O + N	; {@NHOH}	{}
NH2O	= 2H + O + N	; {@NH_2O}	{}
NH2OH	= 3H + O + N	; {@NH_2OH}	{}
LNITROGEN	= N	; {@LNITROGEN}	{lumped N species}

{----- C -----}

{1C (CHO)}			
CH200	= C + 2H + 20	; {@CH_200}	{MCM: carbonyl oxide -
stabilized Criegee Intermediate}			
CH200A	= C + 2H + 20	; {@CH_200^*}	{MCM: carbonyl oxide -
excited Criegee Intermediate}			
CH3	= C + 3H	; {@CH_3}	{methyl radical}
CH30	= C + 3H + 0	; {@CH_30}	{MCM: methoxy radical}
CH302	= C + 3H + 20	; {@CH_30_2}	{MCM: methylperoxy radical}
CH30H	= C + 4H + 0	; {@CH_30H}	{MCM: methanol}
CH300H	= C + 4H + 20	; {@CH_300H}	{MCM: methyl peroxide}
CH4	= C + 4H	; {@CH_4}	{MCM: methane}
CO	= C + 0	; {@CO}	{carbon monoxide}
CO2	= C + 20	; {@CO_2}	{carbon dioxide}
HCHO	= C + 2H + 0	; {@HCHO}	{MCM: methanal =
formaldehyde}			
HC00H	= C + 2H + 20	; {@HC00H}	{MCM: formic acid}
HOCH202	= C + 3H + 30	; {@HOCH_20_2}	{hydroxy methyl peroxy
radical}			
HOCH20H	= C + 4H + 20	; {@HOCH_20H}	{dyhydroxy methane}
HOCH200H	= C + 4H + 30	; {@HOCH_200H}	{hydroxy methyl
hydroperoxide}			
{1C (CHON)}			
CH3N03	= C + 3H + 30 + N	; {@CH_30N0_2}	{MCM: methylnitrate}
CH302N02	= C + 3H + 40 + N	; {@CH_30_2N0_2}	{MCM: peroxy methylnitrate}
CH30N0	= C + 3H + 20 + N	; {@CH_30N0}	{methylnitrite}
CN	= C + N	; {@CN}	{}
HCN	= C + H + N	; {@HCN}	{}
HOCH202N02	= C + 3H + 50 + N	; {@HOCH_20_2N0_2}	{hydroxy methyl peroxy
nitrate}			
NCO	= C + 0 + N	; {@NCO}	{}
{1C (lumped)}			
LCARBON	= C	; {@LCARBON}	{lumped carbon}
{2C (CHO)}			
C2H2	= 2C + 2H	; {@C_2H_2}	{MCM: ethyne}
C2H4	= 2C + 4H	; {@C_2H_4}	{MCM: ethene}
C2H502	= 2C + 5H + 20	; {@C_2H_50_2}	{MCM: ethylperoxy radical}
C2H50H	= 2C + 6H + 0	; {@C_2H_50H}	{MCM: ethanol}
C2H500H	= 2C + 6H + 20	; {@C_2H_500H}	{MCM: ethyl hydro peroxide}
C2H6	= 2C + 6H	; {@C_2H_6}	{MCM: ethane}
CH2CH0H	= 2C + 4H + 0	; {@CH_2CH0H}	{vinyl alcohol}
CH2CO	= 2C + 2H + 0	; {@CH2CO}	{ketene}
CH3CH0	= 2C + 4H + 0	; {@CH_3CH0}	{MCM: acetaldehyde}
CH3CH0H02	= 2C + 5H + 30	; {@CH3CH0H02}	{}
CH3CH0H00H	= 2C + 6H + 30	; {@CH3CH0H00H}	{}
CH3CO	= 2C + 3H + 20	; {@CH_3C(0)}	{acetyl radical}
CH3CO2H	= 2C + 4H + 20	; {@CH_3CO0H}	{MCM: acetic acid}
CH3CO3	= 2C + 3H + 30	; {@CH_3C(0)00}	{MCM: peroxy acetyl radical}
CH3CO3H	= 2C + 4H + 30	; {@CH_3C(0)00H}	{MCM: peroxy acetic acid}
ETHGLY	= 2C + 6H + 20	; {@ETHGLY}	{MCM: HOCH2CH20H}
GLY0X	= 2C + 2H + 20	; {@GLY0X}	{MCM: CHOCHO = glyoxal}
HC0CH202	= 2C + 3H + 30	; {@HC0CH_20_2}	{MCM}
HCOCO	= 2C + H + 20	; {@HCOCO}	{MOM}
HCOCO2H	= 2C + 2H + 30	; {@HCOCO_2H}	{MCM: oxoethanoic acid}
HCOCO3	= 2C + H + 40	; {@HCOCO_3}	{MCM}
HCOCO3H	= 2C + 2H + 40	; {@HCOCO_3H}	{MCM}
HOCH2CH20	= 2C + 5H + 20	; {@HOCH_2CH_20}	{MCM: (2-
hydroxyethyl)oxidanyl}			
HOCH2CH202	= 2C + 5H + 30	; {@HOCH_2CH_20_2}	{MCM: (2-
hydroxyethyl)dioxidanyl}			
HOCH2CHO	= 2C + 4H + 20	; {@HOCH_2CHO}	{MCM: glycolaldehyde}
HOCH2CO	= 2C + 3H + 20	; {@HOCH2CO}	{}
HOCH2CO2H	= 2C + 4H + 30	; {@HOCH_2CO_2H}	{MCM: hydroxyethanoic acid}
HOCH2CO3	= 2C + 3H + 40	; {@HOCH_2CO_3}	{MCM}
HOCH2CO3H	= 2C + 4H + 40	; {@HOCH_2CO_3H}	{MCM}
HOCHCHO	= 2C + 3H + 20	; {@HOCHCHO}	{}
H00CH2CHO	= 2C + 4H + 30	; {@H00CH2CHO}	{}

H00CH2C02H	= 2C + 4H + 40	; {@H00CH2C02H}	{}
H00CH2C03	= 2C + 3H + 50	; {@H00CH_2C0_3}	{}
H00CH2C03H	= 2C + 4H + 50	; {@H00CH2C03H}	{}
HYETH02H	= 2C + 6H + 30	; {@HYETH02H}	{MCM: HOCH2CH200H}
{2C (CH0N)}			
C2H5N03	= 2C + 5H + 30 + N	; {@C_2H_5NO_2}	{MCM: ethyl nitrate}
C2H502N02	= 2C + 5H + 40 + N	; {@C_2H_5O_2NO_2}	{ethyl peroxy nitrate}
CH3CN	= 2C + 3H + N	; {@CH_3CN}	{acetonitrile}
ETH0HN03	= 2C + 5H + 40 + N	; {@ETH0HN03}	{MCM: HOCH2CH20N02}
NCCH202	= 2C + 2H + 20 + N	; {@NCCH_2O_2}	{}
N03CH2CHO	= 2C + 3H + 40 + N	; {@NO_3CH2CHO}	{MCM}
N03CH2C03	= 2C + 2H + 60 + N	; {@NO_3CH2CO_3}	{MCM}
N03CH2PAN	= 2C + 2H + 80 + 2N	; {@NO_3CH2CHO}	{MCM}
PAN	= 2C + 3H + 50 + N	; {@PAN}	{MCM: CH3C(0)00N02 =
peroxyacetylnitrate}			
PHAN	= 2C + 3H + 60 + N	; {@PHAN}	{MCM: HOCH2C(0)00N02}
{3C (CH0)}			
ACET0L	= 3C + 6H + 20	; {@CH_3COCH_2OH}	{MCM: HO-CH2-CO-CH3 =
hydroxy acetone}			
ALCOCH200H	= 3C + 4H + 40	; {@HCOCH200H}	{MCM}
C2H5CHO	= 3C + 6H + 0	; {@C_2H_5CHO}	{MCM: propanal}
PROPACID	= 3C + 6H + 20	; {@C_2H_5CO_2H}	{MCM}
C2H5C03	= 3C + 5H + 30	; {@C_2H_5CO_3}	{MCM}
PERPROACID	= 3C + 6H + 30	; {@C_2H_5CO_3H}	{MCM}
C33C0	= 3C + 2H + 30	; {@HCOCH20H}	{MCM}
C3H6	= 3C + 6H	; {@C_3H_6}	{MCM: propene}
C3H8	= 3C + 8H	; {@C_3H_8}	{MCM: propane}
CH3CHC0	= 3C + 4H + 0	; {@CH3CHC0}	{CH3CHC0}
CH3C0CH202	= 3C + 5H + 30	; {@CH_3COCH_2O_2}	{MCM: peroxyradical from
acetone}			
CH3C0CH3	= 3C + 6H + 0	; {@CH_3COCH_3}	{MCM: acetone}
CH3C0C02H	= 3C + 4H + 30	; {@CH_3COCO_2H}	{MCM: pyruvic acid}
CH3C0C03	= 3C + 3H + 40	; {@CH_3COCO_3}	{MCM}
CH3C0C03H	= 3C + 4H + 40	; {@CH_3COCO_3H}	{MCM}
CH0C0CH202	= 3C + 3H + 40	; {@HCOCH2O_2}	{MCM}
HCOCH2CHO	= 3C + 4H + 30	; {@HCOCH2CHO}	{MCM}
HCOCH2C02H	= 3C + 4H + 40	; {@HCOCH2C02H}	{MCM}
HCOCH2C03	= 3C + 3H + 50	; {@HCOCH2C03}	{MCM}
HCOCH2C03H	= 3C + 4H + 50	; {@HCOCH2C03H}	{MCM}
HCOC0CH200H	= 3C + 4H + 40	; {@HCOCH200H}	{}
HOC2H4C02H	= 3C + 6H + 30	; {@HOC2H4C02H}	{MCM: 3-hydroxypropanoic
acid}			
HOC2H4C03	= 3C + 5H + 40	; {@HOC_2H_4CO_3}	{MCM}
HOC2H4C03H	= 3C + 6H + 40	; {@HOC2H4C03H}	{MCM}
HOCH2C0CH202	= 3C + 5H + 40	; {@HOCH2C0CH202}	{}
HOCH2C0CH200H	= 3C + 6H + 40	; {@HOCH2C0CH200H}	{}
HOCH2C0CHO	= 3C + 4H + 30	; {@HOCH2C0CHO}	{MCM: hydroxypyruvaldehyde}
HYPERACET	= 3C + 6H + 30	; {@CH_3COCH_2O_2H}	{MCM: hydroperoxide from
CH3C0CH202}			
HYPROP02	= 3C + 7H + 30	; {@HYPROP02}	{MCM: CH3CH(02)CH20H}
HYPROP02H	= 3C + 8H + 30	; {@HYPROP02H}	{MCM: CH3CH(00H)CH20H}
IC3H702	= 3C + 7H + 20	; {@iC_3H_7O_2}	{MCM: isopropylperoxy
radical}			
IC3H700H	= 3C + 8H + 20	; {@iC_3H_700H}	{MCM: isopropyl hydro
peroxide}			
IPROP0L	= 3C + 8H + 0	; {@IPROP0L}	{MCM: isopropyl alcohol}
MGLY0X	= 3C + 4H + 20	; {@MGLY0X}	{MCM: CH3COCHO =
methylglyoxal}			
NC3H702	= 3C + 7H + 20	; {@C_3H_7O_2}	{MCM: propylperoxy radical}
NC3H700H	= 3C + 8H + 20	; {@C_3H_700H}	{MCM: propyl hydro peroxide}
NPROP0L	= 3C + 8H + 0	; {@NPROP0L}	{MCM: n-propyl alcohol}
PROPENOL	= 3C + 6H + 0	; {@CH_2CHCH_2OH}	{}
{3C (CH0) aromatics}			
C320H13C0	= 3C + 4H + 30	; {@C320H13C0}	{MCM: hydroxymalonaldehyde}
C3DIAL02	= 3C + 3H + 40	; {@C3DIAL02}	{MCM}
C3DIAL00H	= 3C + 4H + 40	; {@C3DIAL00H}	{MCM}
HCOC0HC03	= 3C + 3H + 50	; {@HCOCH20H}	{MCM}
HCOC0HC03H	= 3C + 4H + 50	; {@HCOCH20H}	{MCM}
METACETHO	= 3C + 4H + 30	; {@METACETHO}	{MCM: acetic formic

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anhydride}
{3C (CHON)}
C3PAN1      = 3C + 5H + 60 + N ; {@C_3PAN1}      {MCM}
C3PAN2      = 3C + 3H + 60 + N ; {@C_3PAN2}      {MCM}
CH3COCH2O2N02 = 3C + 5H + 50 + N ; {@CH_3COCH_2O2N0_2} {CH3-C(0)-CH2-O2N02}
IC3H7N03    = 3C + 7H + 30 + N ; {@iC_3H_7ONO_2}  {MCM: isopropyl nitrate}
NC3H7N03    = 3C + 7H + 30 + N ; {@C_3H_7ONO_2}  {MCM: propyl nitrate}
NOA         = 3C + 5H + 40 + N ; {@NOA}           {MCM: CH3-CO-CH2ON02 =
nitro-oxy-acetone}
PPN         = 3C + 5H + 50 + N ; {@PPN}           {MCM: CH3CH2C(0)O2N02}
PR2O2HN03   = 3C + 7H + 50 + N ; {@PR2O2HN03}     {MCM: CH3-CH(OOH)-CH2ON02}
PRON03B02   = 3C + 6H + 50 + N ; {@PRON03B02}     {MCM: CH3-CH(O2)-CH2ON02}
PROPOLN03   = 3C + 7H + 40 + N ; {@PROPOLN03}     {MCM: HOCH2-CH(CH3)ON02}}
{3C (CHON) aromatics}
HCOCOHPAN   = 3C + 3H + 70 + N ; {@HCOCOHPAN}     {MCM}
{4C (CHO)}
BIACET      = 4C + 6H + 20      ; {@BIACET}      {MCM: CH3-CO-CO-CH3}
BIACET02    = 4C + 5H + 40      ; {@CH_3COCOCH_2O_2} {MCM}
BIACET0H    = 4C + 6H + 30      ; {@BIACET0H}    {MCM: CH3-CO-CO-CH2OH}
BIACET00H   = 4C + 6H + 40      ; {@CH_3COCOCH_2OOH} {MCM}
BUT1ENE     = 4C + 8H           ; {@BUT1ENE}     {MCM}
BUT20L0     = 4C + 8H + 30      ; {@BUT20L0}     {MCM}
BUT20L02    = 4C + 9H + 20      ; {@BUT20L02}    {MCM}
BUT20L00H   = 4C + 10H + 30     ; {@BUT20L00H}   {MCM}
BUTEN0L     = 4C + 8H + 0       ; {@BUTEN0L}     {CH3CH2CHCHOH}
C312C0C03  = 4C + 3H + 50      ; {@C312C0C03}   {MCM}
C312C0C03H  = 4C + 4H + 50      ; {@C312C0C03H}  {MCM}
C3H7CHO     = 4C + 8H + 0       ; {@C_3H_7CHO}    {MCM: n-butanal}
C413C000H   = 4C + 6H + 40      ; {@C413C000H}   {MCM}
C4402       = 4C + 5H + 50      ; {@C4402}       {MCM}
C4400H      = 4C + 6H + 50      ; {@C4400H}      {MCM}
C4CODIAL    = 4C + 4H + 30      ; {@C4CODIAL}    {MCM}
CBUT2ENE    = 4C + 8H           ; {@CBUT2ENE}    {MCM}
CH3COCHCO   = 4C + 4H + 20      ; {@CH_3COCHCO}   {}
CH3COCHO2CHO = 4C + 5H + 40      ; {@CH_3COCHO_2CHO} {}
CH3COCOC02H = 4C + 6H + 40      ; {@CH3COCOC02H}  {}
CH3COOHCHCHO = 4C + 6H + 30      ; {@CH_3COOHCHCHO} {}
CHOC3C002   = 4C + 5H + 40      ; {@CHOC3C002}   {MCM}
CO23C3CHO   = 4C + 4H + 30      ; {@CH_3COC0CHO}  {MCM}
CO2C3CHO    = 4C + 6H + 20      ; {@CO2C3CHO}     {MCM: CH3COCH2CHO}
CO2H3CHO    = 4C + 5H + 30      ; {@CO2H3CHO}     {MCM: CH3-CO-CH(OH)-CHO}
CO2H3C02H   = 4C + 6H + 50      ; {@CO2H3C02H}    {}
CO2H3C03    = 4C + 5H + 50      ; {@CO2H3C03}     {MCM: CH3-CO-CH(OH)-C(0)O2}
CO2H3C03H   = 4C + 6H + 50      ; {@CO2H3C03H}    {MCM: CH3-CO-CH(OH)-C(0)OOH}
EZCH3C02CHCHO = 4C + 5H + 30      ; {@EZCH3C02CHCHO} {}
EZCH0CCH3CHO2 = 4C + 5H + 30      ; {@EZCH0CCH3CHO2} {}
HCOCCCH3CHO0H = 4C + 6H + 30      ; {@HCOCCCH_3CHO0H} {}
HCOCCCH3CO   = 4C + 4H + 20      ; {@HCOCCCH_3CO}  {}
HCOCO2CH3CHO = 4C + 5H + 40      ; {@HCOCO_2CH_3CHO} {}
HMAC        = 4C + 6H + 20      ; {@HMAC}         {MCM: HCOC(CH3)CHOH}
H012C03C4   = 4C + 8H + 30      ; {@H012C03C4}   {MCM: CH3-CO-CH(OH)-CH2OH}
HVMK        = 4C + 6H + 20      ; {@HVMK}         {MCM: CH3COCHCHOH = hydroxy
vinyl methyl ketone}
IBUTALOH    = 4C + 8H + 20      ; {@IBUTALOH}     {MCM}
IBUTDIAL    = 4C + 6H + 20      ; {@IBUTDIAL}     {MCM: HCOC(CH3)CHO}
IBUT0LB02   = 4C + 9H + 20      ; {@IBUT0LB02}    {MCM}
IBUT0LB00H  = 4C + 10H + 30     ; {@IBUT0LB00H}   {}
IC4H10      = 4C + 10H          ; {@iC_4H_<10>}    {MCM: (CH3)3-CH = i-butane}
IC4H902     = 4C + 9H + 20      ; {@IC_4H_9O_2}   {MCM: (CH3)2-CHCH2O2}
IC4H902}
IC4H900H    = 4C + 10H + 20     ; {@IC_4H_9OOH}   {MCM: (CH3)2-CHCH2OOH MCM:
IC4H900H}
IPRCHO      = 4C + 8H + 0       ; {@IPRCHO}       {MCM: (CH3)2CHCHO MCM :
methylpropanal}
IPRC03      = 4C + 7H + 30      ; {@IPRC03}       {MCM: (CH3)2CHC03}
IPRHOC02H   = 4C + 8H + 30      ; {@IPRHOC02H}    {MCM}
IPRHOC03    = 4C + 7H + 40      ; {@IPRHOC03}     {MCM}
IPRHOC03H   = 4C + 8H + 40      ; {@IPRHOC03H}    {MCM}
MAC02       = 4C + 5H + 20      ; {@MAC02}        {}

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MAC02H	= 4C + 6H + 20	; {@MAC02H}	{MCM: CH ₂ =C(CH ₃)COOH =
methacrylic acid}			
MAC03	= 4C + 5H + 30	; {@MAC03}	{MCM: CH ₂ =C(CH ₃)C(O)O ₂ }
MAC03H	= 4C + 6H + 30	; {@MAC03H}	{MCM: CH ₂ =C(CH ₃)C(O)OOH}
MACR	= 4C + 6H + 0	; {@MACR}	{MCM: CH ₂ =C(CH ₃)CHO =
methacrolein}			
MACR0	= 4C + 7H + 30	; {@MACR0}	{MCM}
MACR02	= 4C + 7H + 40	; {@MACR02}	{MCM: HOCH ₂ C(OO)(CH ₃)CHO}
MACR0H	= 4C + 8H + 30	; {@MACR0H}	{MCM: HOCH ₂ C(OH)(CH ₃)CHO}
MACR00H	= 4C + 8H + 40	; {@MACR00H}	{MCM: HOCH ₂ C(OOH)(CH ₃)CHO}
MB000	= 4C + 8H + 30	; {@MB000}	{MCM}
MEK	= 4C + 8H + 0	; {@MEK}	{MCM: CH ₃ -CO-CH ₂ -CH ₃ =
methyl ethyl ketone}			
MEPROPENE	= 4C + 8H	; {@MEPROPENE}	{MCM}
MPROPENOL	= 4C + 8H + 0	; {@MPROPENOL}	{(CH ₃) ₂ CHOH methylpropenol}
MVK	= 4C + 6H + 0	; {@MVK}	{MCM: CH ₃ -CO-CH=CH ₂ =
methyl vinyl ketone}			
NC4H10	= 4C + 10H	; {@C_4H_<10>}	{MCM: CH ₃ -CH ₂ -CH ₂ -CH ₃ = n-
butane}			
PERIBUACID	= 4C + 8H + 30	; {@PERIBUACID}	{MCM: (CH ₃) ₂ CHCO ₃ H}
TBUT2ENE	= 4C + 8H	; {@TBUT2ENE}	{MCM}
TC4H902	= 4C + 9H + 20	; {@TC_4H_90_2}	{MCM: (CH ₃) ₃ -CO ₂ }
TC4H900H	= 4C + 10H + 20	; {@TC_4H_900H}	{MCM: (CH ₃) ₃ -COOH}
{4C (CH ₀) aromatics}			
BZFUC0	= 4C + 4H + 40	; {@BZFUC0}	{MCM}
BZFU02	= 4C + 5H + 30	; {@BZFU02}	{MCM}
BZFU0NE	= 4C + 4H + 20	; {@BZFU0NE}	{MCM: 2(5H)-furanone}
BZFU00H	= 4C + 6H + 50	; {@BZFU00H}	{MCM}
C01403CHO	= 4C + 4H + 40	; {@C01403CHO}	{MCM}
C01403C02H	= 4C + 4H + 50	; {@C01403C02H}	{MCM}
C02C4DIAL	= 4C + 2H + 40	; {@C02C4DIAL}	{MCM: 2,3-
dioxosuccinaldehyde}			
EPXC4DIAL	= 4C + 4H + 30	; {@EPXC4DIAL}	{MCM}
EPXDLC02H	= 4C + 4H + 40	; {@EPXDLC02H}	{MCM}
EPXDLC03	= 4C + 3H + 50	; {@EPXDLC03}	{MCM}
EPXDLC03H	= 4C + 4H + 50	; {@EPXDLC03H}	{MCM}
HOCOC4DIAL	= 4C + 4H + 40	; {@HOCOC4DIAL}	{MCM: 2-hydroxy-3-
oxosuccinaldehyde}			
MALANHY	= 4C + 2H + 30	; {@MALANHY}	{MCM: maleic anhydride}
MALANHY02	= 4C + 3H + 60	; {@MALANHY02}	{MCM}
MALANHY00H	= 4C + 4H + 60	; {@MALANHY00H}	{MCM}
MALDALC02H	= 4C + 4H + 30	; {@MALDALC02H}	{MCM: 4-oxo-2-butenic acid}
MALDALC03H	= 4C + 4H + 40	; {@MALDALC03H}	{MCM}
MALDIAL	= 4C + 4H + 20	; {@MALDIAL}	{MCM: 2-butenedial}
MALDIALC03	= 4C + 3H + 40	; {@MALDIALC03}	{MCM}
MALDIAL02	= 4C + 5H + 50	; {@MALDIAL02}	{MCM}
MALDIAL00H	= 4C + 6H + 50	; {@MALDIAL00H}	{MCM}
MALNHYOHC0	= 4C + 2H + 50	; {@MALNHYOHC0}	{MCM}
MECOACE00H	= 4C + 6H + 50	; {@MECOACE00H}	{MCM}
MECOACETO2	= 4C + 5H + 50	; {@MECOACETO2}	{MCM}
{4C (CH ₀ N)}			
BUT20LN03	= 4C + 9H + 50 + N	; {@BUT20LN03}	{MCM}
C312COPAN	= 4C + 3H + 70 + N	; {@C312COPAN}	{MCM}
C4PAN5	= 4C + 7H + 60 + N	; {@C4PAN5}	{MCM}
IBUTOLBN03	= 4C + 9H + 40 + N	; {@IBUTOLBN03}	{MCM}
IC4H9N03	= 4C + 9H + 30 + N	; {@IC4H9N03}	{MCM}
MACRN03	= 4C + 7H + 50 + N	; {@MACRN03}	{MCM}
MPAN	= 4C + 5H + 50 + N	; {@MPAN}	{MCM: CH ₂ =C(CH ₃)C(O)OON02 =
peroxymethacryloyl nitrate = peroxymethacrylic nitric anhydride}			
MVKN03	= 4C + 7H + 50 + N	; {@MVKN03}	{MCM}
PIPN	= 4C + 7H + 50 + N	; {@PIPN}	{MCM: (CH ₃) ₂ CHCO ₃ }
TC4H9N03	= 4C + 9H + 30 + N	; {@TC4H9N03}	{MCM}
{4C (CH ₀ N) aromatics}			
EPXDLPAN	= 4C + 3H + 70 + N	; {@EPXDLPAN}	{MCM}
MALDIALPAN	= 4C + 3H + 60 + N	; {@MALDIALPAN}	{MCM}
NBZFU02	= 4C + 4H + 70 + N	; {@NBZFU02}	{MCM}
NBZFU0NE	= 4C + 3H + 60 + N	; {@NBZFU0NE}	{MCM}
NBZFU00H	= 4C + 5H + 70 + N	; {@NBZFU00H}	{MCM}
NC4DC02H	= 4C + 3H + 50 + N	; {@NC4DC02H}	{MCM}

{4C (CH0) (lumped)}		
LBUT1EN02	= 4C + 9H + 20	; {@LBUT1EN02} {H03C402 + NBUTOLA02}
LBUT1EN00H	= 4C + 10H + 30	; {@LBUT1EN00H} {H03C400H + NBUTOLA00H}
LC4H902	= 4C + 9H + 20	; {@LC_4H_90_2} {CH3-CH2-CH(02)-CH3 + CH3-
CH2-CH2-CH202 = NC4H902 + SC4H902}		
LC4H900H	= 4C + 10H + 20	; {@LC_4H_900H} {CH3-CH2-CH(00H)-CH3 + CH3-
CH2-CH2-CH200H = NC4H900H + SC4H900H}		
LHMKAB02	= 4C + 7H + 40	; {@LHMKAB02} {HOCH2-CH(02)-CO-CH3 +
CH2(02)-CH(OH)-CO-CH3}		
LHMKAB00H	= 4C + 8H + 40	; {@LHMKAB00H} {HOCH2-CH(00H)-CO-CH3 +
CH2(00H)-CH(OH)-CO-CH3}		
LMEK02	= 4C + 7H + 30	; {@LMEK02} {CH3-CO-CH2-CH2-00 + CH3-CO-
CH(02)-CH3}		
LMEK00H	= 4C + 8H + 30	; {@LMEK00H} {CH3-CO-CH2-CH2-00H + CH3-
CO-CH(00H)-CH3}		
{4C (CH0N) (lumped)}		
LBUT1ENN03	= 4C + 9H + 50 + N	; {@LBUT1ENN03} {H03C4N03 + NBUTOLAN03}
LC4H9N03	= 4C + 9H + 30 + N	; {@LC4H9N03} {NC4H9N03 + SC4H9N03}
LMEKN03	= 4C + 7H + 50 + N	; {@LMEKN03} {CH3-CO-CH2-CH2-0N02 + CH3-
CO-CH(0N02)-CH3}		
{5C (CH0)}		
C10DC202C40D	= 5C + 7H + 40	; {@C10DC202C40D} {}
C10DC202C400H	= 5C + 9H + 50	; {@C10DC202C400H} {}
C10DC200HC40D	= 5C + 8H + 40	; {@C10DC200HC40D} {}
C10DC302C400H	= 5C + 9H + 50	; {@C10DC302C400H} {}
C100HC202C40D	= 5C + 9H + 50	; {@C100HC202C40D} {}
C100HC200HC40D	= 5C + 10H + 50	; {@C100HC200HC40D} {}
C100HC302C40D	= 5C + 9H + 50	; {@C100HC302C40D} {}
C4MDIAL	= 5C + 6H + 20	; {@C4MDIAL} {MCM: 2-methyl-butenedial}
C51102	= 5C + 7H + 40	; {@C51102} {MCM}
C51100H	= 5C + 8H + 40	; {@C51100H} {MCM}
C51202	= 5C + 7H + 40	; {@C51202} {MCM}
C51200H	= 5C + 8H + 40	; {@C51200H} {MCM}
C513C0	= 5C + 6H + 40	; {@C513C0} {MCM}
C51302	= 5C + 7H + 50	; {@C51302} {MCM}
C51300H	= 5C + 8H + 50	; {@C51300H} {MCM}
C51402	= 5C + 7H + 40	; {@C51402} {MCM}
C51400H	= 5C + 8H + 40	; {@C51400H} {MCM}
C5902	= 5C + 9H + 50	; {@C5902} {MCM: HOCH2-CO-C(CH3)(02)-
CH20H}		
C5900H	= 5C + 10H + 50	; {@C5900H} {MCM: HOCH2-CO-C(CH3)(00H)-
CH20H}		
C5H8	= 5C + 8H	; {@C_5H_8} {MCM: CH2=C(CH3)CH=CH2 =
isoprene}		
CHOC3C0C03	= 5C + 5H + 50	; {@CHOC3C0C03} {MCM}
CHOC3C000H	= 5C + 6H + 40	; {@CHOC3C000H} {MCM}
C013C4CH0	= 5C + 6H + 30	; {@C013C4CH0} {MCM}
C023C4CH0	= 5C + 6H + 30	; {@C023C4CH0} {MCM}
C023C4C03	= 5C + 5H + 50	; {@C023C4C03} {MCM}
C023C4C03H	= 5C + 6H + 50	; {@C023C4C03H} {MCM}
DB10	= 5C + 9H + 30	; {@DB102} {Alkoxy radical which
undergoes the double H-shift predicted by T. Dibble and confirmed by F. Paulot}		
DB102	= 5C + 9H + 40	; {@DB102} {Peroxy radical with a
vinyl alcohol part}		
DB100H	= 5C + 10H + 40	; {@DB100H} {}
DB202	= 5C + 9H + 50	; {@DB102} {}
DB200H	= 5C + 10H + 50	; {@DB200H} {}
HC0C5	= 5C + 8H + 20	; {@HC0C5} {MCM: HOCH2-CO-C(CH3)=CH2}
ISOPA0H	= 5C + 10H + 20	; {@ISOPA0H} {MCM: HOCH2-C(CH3)=CH-CH20H}
ISOPB02	= 5C + 9H + 30	; {@ISOPB02} {MCM: HOCH2-C(CH3)(02)-
CH=CH2}		
ISOPB0H	= 5C + 10H + 20	; {@ISOPB0H} {MCM: HOCH2-C(CH3)(0H)-
CH=CH2}		
ISOPB00H	= 5C + 10H + 30	; {@ISOPB00H} {MCM: HOCH2-C(CH3)(00H)-
CH=CH2}		
ISOPD02	= 5C + 9H + 30	; {@ISOPD02} {MCM: CH2=C(CH3)CH(02)-
CH20H}		
ISOPD0H	= 5C + 10H + 20	; {@ISOPD0H} {MCM: CH2=C(CH3)CH(0H)-
CH20H}		

ISOPD00H	= 5C + 10H + 30	; {@ISOPD00H}	{MCM: CH ₂ =C(CH ₃)CH(OOH) -
CH ₂ OH}			
MBO	= 5C + 10H + 0	; {@MBO}	{MCM: 2-methyl-3-buten-2-ol}
MBOACO	= 5C + 10H + 30	; {@MBOACO}	{MCM}
MBOCOCO	= 5C + 8H + 30	; {@MBOCOCO}	{MCM}
ME3FURAN	= 5C + 6H + 0	; {@3METHYLFURAN}	{3-methyl-furan}
{5C aromatics (CH ₀)}			
ACCOMETCHO	= 5C + 6H + 40	; {@ACCOMETCHO}	{MCM}
ACCOMEC03	= 5C + 5H + 60	; {@ACCOMEC03}	{MCM}
ACCOMEC03H	= 5C + 6H + 60	; {@ACCOMEC03H}	{MCM}
C2403CC02H	= 5C + 6H + 50	; {@C2403CC02H}	{MCM}
C4C02DBC03	= 5C + 3H + 50	; {@C4C02DBC03}	{MCM}
C4C02DC03H	= 5C + 4H + 50	; {@C4C02DC03H}	{MCM}
C5134C02OH	= 5C + 6H + 40	; {@C5134C02OH}	{MCM: 2-hydroxy-3,4-
dioxopentanal}			
C54C0	= 5C + 4H + 40	; {@C54C0}	{MCM: 2,3,4-trioxopentanal}
C5C01402	= 5C + 5H + 40	; {@C5C01402}	{MCM}
C5C0140H	= 5C + 6H + 30	; {@C5C0140H}	{MCM: 4-oxo-2-pentenoic
acid}			
C5C01400H	= 5C + 6H + 40	; {@C5C01400H}	{MCM}
C5DIALC0	= 5C + 4H + 30	; {@C5DIALC0}	{MCM}
C5DIAL02	= 5C + 5H + 40	; {@C5DIAL02}	{MCM}
C5DIAL00H	= 5C + 6H + 40	; {@C5DIAL00H}	{MCM}
C5DICARB	= 5C + 6H + 20	; {@C5DICARB}	{MCM: 4-oxo-2-pentenal}
C5DICARB02	= 5C + 7H + 50	; {@C5DICARB02}	{MCM:
carboxy(hydroxy)acetate}			
C5DICAR00H	= 5C + 8H + 50	; {@C5DICAR00H}	{MCM}
MC30DBC02H	= 5C + 6H + 30	; {@MC30DBC02H}	{MCM}
MMALANHY	= 5C + 4H + 30	; {@MMALANHY}	{MCM: 3-methyl-2,5-
furandione}			
MMALANHY02	= 5C + 5H + 60	; {@MMALANHY02}	{MCM}
MMALNHY00H	= 5C + 6H + 60	; {@MMALNHY00H}	{MCM}
TLFU02	= 5C + 7H + 50	; {@TLFU02}	{MCM}
TLFU0NE	= 5C + 6H + 20	; {@TLFU0NE}	{MCM: 5-methyl-2(5H) -
furanone}			
TLFU00H	= 5C + 8H + 50	; {@TLFU00H}	{MCM}
{5C (CHON)}			
C4MCON030H	= 5C + 9H + 50 + N	; {@C4MCON030H}	{MCM}
C514N03	= 5C + 7H + 50 + N	; {@C514N03}	{MCM}
C5PAN9	= 5C + 5H + 70 + N	; {@C5PAN9}	{MCM}
CHOC3COPAN	= 5C + 5H + 50 + N	; {@CHOC3COPAN}	{MCM}
DB1N03	= 5C + 9H + 60 + N	; {@DB1N03}	{}
ISOPBDN0302	= 5C + 10H + 70 + N	; {@ISOPBDN0302}	{}
ISOPBN03	= 5C + 9H + 40 + N	; {@ISOPBN03}	{MCM: HOCH ₂ -C(CH ₃)(ON02) -
CH=CH ₂ }			
ISOPDN03	= 5C + 9H + 40 + N	; {@ISOPDN03}	{MCM: CH ₂ =C(CH ₃)CH(ON02) -
CH ₂ OH}			
NC4CH0	= 5C + 7H + 40 + N	; {@NC4CH0}	{MCM: O ₂ N0CH ₂ -C(CH ₃)=CH-CH0}
NC40HC03	= 5C + 8H + 60 + N	; {@NC40HC03}	{MCM}
NC40HC03H	= 5C + 9H + 60 + N	; {@NC40HC03H}	{MCM}
NC40HCPAN	= 5C + 8H + 80 + 2N	; {@NC40HCPAN}	{MCM}
NISOP02	= 5C + 8H + 50 + N	; {@NISOP02}	{MCM: O ₂ N0CH ₂ -C(CH ₃)=CH-
CH ₂ O ₂ }			
NISOP00H	= 5C + 9H + 50 + N	; {@NISOP00H}	{MCM: O ₂ N0CH ₂ -C(CH ₃)=CH-
CH ₂ OOH}			
NMBOBCO	= 5C + 9H + 50 + N	; {@NMBOBCO}	{MCM}
{5C aromatics (CHON)}			
ACCOMEPAN	= 5C + 5H + 60 + N	; {@ACCOMEPAN}	{MCM}
C4C02DBPAN	= 5C + 3H + 70 + N	; {@C4C02DBPAN}	{MCM}
C5C002N02	= 5C + 5H + 60 + N	; {@C5C002N02}	{MCM}
NC4MDC02H	= 5C + 5H + 50 + N	; {@NC4MDC02H N}	{MCM}
NTLFU02	= 5C + 6H + 70 + N	; {@NTLFU02}	{MCM}
NTLFU00H	= 5C + 7H + 60 + N	; {@NTLFU00H}	{MCM}
{5C (CH ₀) (lumped)}			
LC57802	= 5C + 9H + 50	; {@LC57802}	{HOCH ₂ -CH(OH)C(CH ₃)(O ₂)-CHO
+ HOCH ₂ -C(CH ₃)(O ₂)-CH(OH)-CH ₀ }			
LC57800H	= 5C + 10H + 50	; {@LC57800H}	{HOCH ₂ -CH(OH)C(CH ₃)(OOH) -
CHO + HOCH ₂ -C(CH ₃)(OOH)-CH(OH)-CH ₀ }			
LDISOPACO	= 5C + 9H + 20	; {@LDISOPACO}	{}

LDISOPAC02	= 5C + 9H + 30	; {@LDISOPAC02}	{}
LHC4ACCHO	= 5C + 8H + 20	; {@LHC4ACCHO}	{HOCH2-C(CH3)=CH-CHO +
HOCH2-CH=C(CH3)-CHO}			
LHC4ACC02H	= 5C + 8H + 30	; {@LHC4ACC02H}	{HOCH2-C(CH3)=CH-C(O)OH +
HOCH2-CH=C(CH3)-C(O)OH}			
LHC4ACC03	= 5C + 7H + 40	; {@LHC4ACC03}	{HOCH2-C(CH3)=CH-C(O)O2 +
HOCH2-CH=C(CH3)-C(O)O2}			
LHC4ACC03H	= 5C + 8H + 40	; {@LHC4ACC03H}	{HOCH2-C(CH3)=CH-C(O)OOH +
HOCH2-CH=C(CH3)-C(O)OOH}			
LIEPOX	= 5C + 10H + 30	; {@LIEPOX}	{epoxydiol}
LISOPAB	= 5C + 9H + 0	; {@LISOPAB}	{}
LISOPACO	= 5C + 9H + 20	; {@LISOPACO}	{HOCH2-C(CH3)=CH-CH2O +
HOCH2-CH=C(CH3)-CH2O}			
LISOPAC02	= 5C + 9H + 30	; {@LISOPAC02}	{HOCH2-C(CH3)=CH-CH2O2 +
HOCH2-CH=C(CH3)-CH2O2}			
LISOPAC00H	= 5C + 10H + 30	; {@LISOPAC00H}	{HOCH2-C(CH3)=CH-CH2OOH +
HOCH2-CH=C(CH3)-CH2OOH}			
LISOPCD	= 5C + 9H + 0	; {@LISOPCD}	{}
LISOPEF0	= 5C + 9H + 20	; {@LISOPEF0}	{}
LISOPEF02	= 5C + 9H + 30	; {@LISOPEF02}	{}
LMBOAB02	= 5C + 11H + 40	; {@LMBOAB02}	{}
LMBOAB00H	= 5C + 12H + 40	; {@LMBOAB00H}	{}
LME3FURAN02	= 5C + 7H + 40	; {@L3METHYLFURAN02}	{hydroxy-3-methyl-furan
peroxy radical}			
LZC03C23DBC0D	= 5C + 5H + 40	; {@LZC03C23DBC0D}	{}
LZC03HC23DBC0D	= 5C + 6H + 40	; {@LZC03HC23DBC0D}	{C5PACALD1 + C5PACALD2}
LZC0DC23DBC00H	= 5C + 8H + 30	; {@LZC0DC23DBC00H}	{C5HPALD1 + C5HPALD2}
{5C (CHON) (lumped)}			
LC5PAN1719	= 5C + 7H + 60 + N	; {@LC5PAN1719}	{HOCH2-C(CH3)=CH-C(O)OON02
+ HOCH2-CH=C(CH3)C(O)OON02}			
LISOPACN03	= 5C + 9H + 40 + N	; {@LISOPACN03}	{HOCH2-C(CH3)=CH-CH2ON02 +
HOCH2-CH=C(CH3)-CH2ON02}			
LISOPACN0302	= 5C + 10H + 70 + N	; {@LISOPACN0302}	{R02 resulting from OH-
addition to ISOPAN03 and ISOPCN03}			
LMBOABN03	= 5C + 11H + 50 + N	; {@LMBOABN03}	{}
LNIS03	= 5C + N	; {@LNIS03}	{C51002+NC4C03 = CHO-CH(OH) -
C(CH3)(O2)-CH2ON02 + 02NOCH2-C(CH3)=CH-C(O)O2}			
LNIS00H	= 5C + N	; {@LNIS00H}	{CHO-CH(OH)-C(CH3)(OOH) -
CH2ON02 + 02NOCH2-C(CH3)=CH-C(O)OOH}			
LNMB0AB02	= 5C + 9H + 60 + N	; {@LNMB0AB02}	{}
LNMB0AB00H	= 5C + 10H + 60 + N	; {@LNMB0AB00H}	{}
LZCPANC23DBC0D	= 5C + 5H + 60 + N	; {@LZCPANC23DBC0D}	{}
{6C (CHO)}			
C614C0	= 6C + 8H + 40	; {@C614C0}	{MCM}
C61402	= 6C + 9H + 50	; {@C61402}	{MCM}
C61400H	= 6C + 10H + 50	; {@C61400H}	{MCM}
C0235C5CHO	= 6C + 6H + 40	; {@C0235C5CHO}	{MCM}
C0235C602	= 6C + 7H + 50	; {@C0235C602}	{MCM}
C0235C600H	= 6C + 8H + 50	; {@C0235C600H}	{MCM}
{C6 (CHO) aromatics}			
BENZENE	= 6C + 6H	; {@BENZENE}	{MCM}
BZBIPERO2	= 6C + 7H + 50	; {@BZBIPERO2}	{MCM}
BZBIPERO0H	= 6C + 8H + 50	; {@BZBIPERO0H}	{MCM}
BZEMUCC0	= 6C + 6H + 50	; {@BZEMUCC0}	{MCM}
BZEMUCC02H	= 6C + 6H + 40	; {@BZEMUCC02H}	{MCM}
BZEMUCC03	= 6C + 5H + 50	; {@BZEMUCC03}	{MCM}
BZEMUCC03H	= 6C + 6H + 50	; {@BZEMUCC03H}	{MCM}
BZEMUC02	= 6C + 7H + 60	; {@BZEMUC02}	{MCM}
BZEMUC00H	= 6C + 8H + 60	; {@BZEMUC00H}	{MCM}
BZEPOXMUC	= 6C + 6H + 30	; {@BZEPOXMUC}	{MCM}
BZOBIPEROH	= 6C + 6H + 40	; {@BZOBIPEROH}	{MCM}
C5C02DBC03	= 6C + 5H + 50	; {@C5C02DBC03}	{MCM}
C5C02DC03H	= 6C + 6H + 50	; {@C5C02DC03H}	{MCM}
C5C020HC03	= 6C + 5H + 60	; {@C5C020HC03}	{MCM}
C5C00HC03H	= 6C + 6H + 60	; {@C5C00HC03H}	{MCM}
C6125C0	= 6C + 6H + 30	; {@C6125C0}	{MCM: 2,5-dioxo-3-hexenal}
C615C0202	= 6C + 7H + 40	; {@C615C0202}	{MCM}
C615C0200H	= 6C + 8H + 40	; {@C615C0200H}	{MCM}
C6C04DB	= 6C + 4H + 40	; {@C6C04DB}	{MCM}

C6H50	= 6C + 5H + 0	; {@C6H50}	{MCM: phenyloxidanyl}
C6H502	= 6C + 5H + 20	; {@C6H502}	{MCM}
C6H500H	= 6C + 6H + 20	; {@C6H500H}	{MCM: phenyl hydroperoxide}
CATEC10	= 6C + 5H + 20	; {@CATEC10}	{MCM: 2- λ 1-oxidanylphenol}
CATEC102	= 6C + 5H + 30	; {@CATEC102}	{MCM}
CATEC100H	= 6C + 6H + 30	; {@CATEC100H}	{MCM}
CATECH0L	= 6C + 4H + 20	; {@CATECH0L}	{MCM: catechol}
CPDKETENE	= 6C + 4H + 0	; {@CPDKETENE}	{hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}			
PBZQCO	= 6C + 4H + 40	; {@PBZQCO}	{MCM}
PBZQ02	= 6C + 5H + 50	; {@PBZQ02}	{MCM}
PBZQ0NE	= 6C + 4H + 20	; {@PBZQ0NE}	{MCM: 1,4-benzoquinone}
PBZQ00H	= 6C + 6H + 50	; {@PBZQ00H}	{MCM}
PHEN02	= 6C + 7H + 60	; {@PHEN02}	{MCM}
PHEN0L	= 6C + 6H + 0	; {@PHEN0L}	{MCM}
PHEN00H	= 6C + 8H + 60	; {@PHEN00H}	{MCM}
{6C (CH0N)}			
C614N03	= 6C + 9H + 60 + N	; {@C614N03}	{MCM}
{C6 (CH0N) aromatics}			
BZBIPERN03	= 6C + 7H + 60 + N	; {@BZBIPERN03}	{MCM}
BZEMUCN03	= 6C + 7H + 70 + N	; {@BZEMUCN03}	{MCM}
BZEMUCPAN	= 6C + 5H + 70 + N	; {@BZEMUCPAN}	{MCM}
C5C02DBPAN	= 6C + 5H + 70 + N	; {@C5C02DBPAN}	{MCM}
C5C020HPAN	= 6C + 5H + 80 + N	; {@C5C020HPAN}	{MCM}
DNPHEN	= 6C + 4H + 50 + 2N	; {@DNPHEN}	{MCM: 2,4-dinitrophenol}
DNPHEN02	= 6C + 5H + 100 + 2N	; {@DNPHEN02}	{MCM}
DNPHEN00H	= 6C + 6H + 100 + 2N	; {@DNPHEN00H}	{MCM}
HOC6H4N02	= 6C + 5H + 30 + N	; {@HOC6H4N02}	{MCM: 2-nitrophenol}
NBZQ02	= 6C + 4H + 70 + N	; {@NBZQ02}	{MCM}
NBZQ00H	= 6C + 5H + 70 + N	; {@NBZQ00H}	{MCM}
NCATECH0L	= 6C + 5H + 40 + N	; {@NCATECH0L}	{MCM}
NCATEC02	= 6C + 6H + 90 + N	; {@NCATEC02}	{MCM}
NCATEC00H	= 6C + 7H + 90 + N	; {@NCATEC00H}	{MCM}
NCPDKETENE	= 6C + 3H + 30 + N	; {@NCPDKETENE}	{hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}			
NDNPHEN02	= 6C + 4H + 120 + 3N	; {@NDNPHEN02}	{MCM}
NDNPHEN00H	= 6C + 5H + 120 + 3N	; {@NDNPHEN00H}	{MCM}
NNCATEC02	= 6C + 5H + 110 + 2N	; {@NNCATEC02}	{MCM}
NNCATEC00H	= 6C + 6H + 110 + 2N	; {@NNCATEC00H}	{MCM}
NPHEN10	= 6C + 4H + 30 + N	; {@NPHEN10}	{MCM}
NPHEN102	= 6C + 4H + 40 + N	; {@NPHEN102}	{MCM}
NPHEN100H	= 6C + 5H + 40 + N	; {@NPHEN100H}	{MCM}
NPHEN02	= 6C + 6H + 80 + N	; {@NPHEN02}	{MCM}
NPHEN00H	= 6C + 7H + 80 + N	; {@NPHEN00H}	{MCM}
{7C (CH0)}			
C235C6C03H	= 7C + 8H + 60	; {@C235C6C03H}	{MCM}
C71602	= 7C + 9H + 50	; {@C71602}	{MCM}
C71600H	= 7C + 10H + 50	; {@C71600H}	{MCM}
C72102	= 7C + 11H + 40	; {@C72102}	{MCM}
C72100H	= 7C + 12H + 40	; {@C72100H}	{MCM}
C72202	= 7C + 11H + 50	; {@C72202}	{MCM}
C72200H	= 7C + 12H + 50	; {@C72200H}	{MCM}
C0235C6CH0	= 7C + 8H + 40	; {@C0235C6CH0}	{MCM}
C0235C6C03	= 7C + 7H + 60	; {@C0235C6C03}	{MCM}
MCPDKETENE	= 7C + 6H + 20	; {@MCPDKETENE}	{hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}			
R006R30	= 7C + 11H + 40	; {@R006R30}	{from ref3019}
R006R302	= 7C + 11H + 50	; {@R006R302}	{R006R300 from ref3019}
R006R502	= 7C + 11H + 70	; {@R006R502}	{R006R500 from ref3019}
{C7 (CH0) aromatics}			
BENZAL	= 7C + 6H + 0	; {@BENZAL}	{MCM}
C6C020HC03	= 7C + 7H + 60	; {@C6C020HC03}	{MCM}
C6C00HC03H	= 7C + 8H + 60	; {@C6C00HC03H}	{MCM}
C6H5CH202	= 7C + 7H + 20	; {@C6H5CH202}	{MCM: benzyldioxidanyl}
C6H5CH200H	= 7C + 8H + 20	; {@C6H5CH200H}	{MCM: benzyl hydroperoxide}
C6H5C03	= 7C + 5H + 30	; {@C6H5C03}	{MCM}
C6H5C03H	= 7C + 6H + 30	; {@C6H5C03H}	{MCM: perbenzoic acid}
C7C04DB	= 7C + 6H + 40	; {@C7C04DB}	{MCM}
CRES02	= 7C + 9H + 60	; {@CRES02}	{MCM}

CRESOL	= 7C + 8H + 0	; {@CRESOL}	{MCM: 2-methylphenol}
CRES00H	= 7C + 10H + 60	; {@CRES00H}	{MCM}
MCATEC10	= 7C + 7H + 20	; {@MCATEC10}	{MCM}
MCATEC102	= 7C + 7H + 30	; {@MCATEC102}	{MCM}
MCATEC100H	= 7C + 8H + 30	; {@MCATEC100H}	{MCM}
MCATECHOL	= 7C + 8H + 20	; {@MCATECHOL}	{MCM: 3-methylcatechol}
OXYL102	= 7C + 7H + 20	; {@OXYL102}	{MCM: 1-methyl-2-(oxo-λ3-
oxidanyl)benzene}			
OXYL100H	= 7C + 8H + 20	; {@OXYL100H}	{MCM}
PHC00H	= 7C + 6H + 20	; {@PHC00H}	{MCM: benzoic acid}
PTLQCO	= 7C + 6H + 40	; {@PTLQCO}	{MCM}
PTLQ02	= 7C + 7H + 50	; {@PTLQ02}	{MCM}
PTLQONE	= 7C + 6H + 20	; {@PTLQONE}	{MCM: 2-methyl-1,4-
benzoquinone}			
PTLQ00H	= 7C + 8H + 50	; {@PTLQ00H}	{MCM}
TLBIPER02	= 7C + 9H + 50	; {@TLBIPER02}	{MCM}
TLBIPER00H	= 7C + 10H + 50	; {@TLBIPER00H}	{MCM}
TLEMUCCO	= 7C + 8H + 50	; {@TLEMUCCO}	{MCM}
TLEMUCC02H	= 7C + 8H + 40	; {@TLEMUCC02H}	{MCM}
TLEMUCC03	= 7C + 7H + 50	; {@TLEMUCC03}	{MCM}
TLEMUCC03H	= 7C + 8H + 50	; {@TLEMUCC03H}	{MCM}
TLEMUC02	= 7C + 9H + 60	; {@TLEMUC02}	{MCM}
TLEMUC00H	= 7C + 10H + 60	; {@TLEMUC00H}	{MCM}
TLEPOXMUC	= 7C + 8H + 30	; {@TLEPOXMUC}	{MCM}
TLOBIPEROH	= 7C + 8H + 40	; {@TLOBIPEROH}	{MCM}
TOL10	= 7C + 7H + 0	; {@TOL10}	{MCM: (2-
methylphenyl)oxidanyl}			
TOLUENE	= 7C + 8H	; {@TOLUENE}	{MCM}
{7C (CHON)}			
C7PAN3	= 7C + 7H + 80 + N	; {@C7PAN3}	{MCM}
{C7 (CHON) aromatics}			
C6C020HPAN	= 7C + 7H + 80 + N	; {@C6C020HPAN}	{MCM}
C6H5CH2N03	= 7C + 7H + 30 + N	; {@C6H5CH2N03}	{MCM: benzyl nitrate}
DNCRES	= 7C + 6H + 50 + 2N	; {@DNCRES}	{MCM: 2-methyl-4,6-
dinitrophenol}			
DNCRES02	= 7C + 7H + 100 + 2N	; {@DNCRES02}	{MCM}
DNCRES00H	= 7C + 8H + 100 + 2N	; {@DNCRES00H}	{MCM}
MNCATECH	= 7C + 7H + 40 + N	; {@MNCATECH}	{MCM: 3-methyl-6-nitro-1,2-
benzenediol}			
MNCATEC02	= 7C + 8H + 90 + N	; {@MNCATEC02}	{MCM}
MNCATEC00H	= 7C + 9H + 90 + N	; {@MNCATEC00H}	{MCM}
MNCPDKETENE	= 7C + 5H + 30 + N	; {@MNCPDKETENE}	{hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}			
MNNCATC00H	= 7C + 8H + 110 + 2N	; {@MNNCATC00H}	{MCM}
MNNCATEC02	= 7C + 7H + 110 + 2N	; {@MNNCATEC02}	{MCM}
NCRES10	= 7C + 6H + 30 + N	; {@NCRES10}	{MCM}
NCRES102	= 7C + 6H + 40 + N	; {@NCRES102}	{MCM}
NCRES100H	= 7C + 7H + 40 + N	; {@NCRES100H}	{MCM}
NCRES02	= 7C + 8H + 80 + N	; {@NCRES02}	{MCM}
NCRES00H	= 7C + 9H + 80 + N	; {@NCRES00H}	{MCM}
NDNCRES02	= 7C + 6H + 20 + 3N	; {@NDNCRES02}	{MCM}
NDNCRES00H	= 7C + 7H + 120 + 3N	; {@NDNCRES00H}	{MCM}
NPTLQ02	= 7C + 6H + 70 + N	; {@NPTLQ02}	{MCM}
NPTLQ00H	= 7C + 7H + 70 + N	; {@NPTLQ00H}	{MCM}
PBZN	= 7C + 5H + 50 + N	; {@PBZN}	{MCM: benzoyl nitro
peroxide}			
TLBIPERN03	= 7C + 9H + 60 + N	; {@TLBIPERN03}	{MCM}
TLEMUCN03	= 7C + 9H + 70 + N	; {@TLEMUCN03}	{MCM}
TLEMUCPAN	= 7C + 7H + 70 + N	; {@TLEMUCPAN}	{MCM}
TOL10HN02	= 7C + 7H + 30 + N	; {@TOL10HN02}	{MCM: 2-methyl-6-
nitrophenol}			
{8C (CHO)}			
C721CHO	= 8C + 12H + 30	; {@C721CHO}	{MCM}
C721C03	= 8C + 11H + 50	; {@C721C03}	{MCM}
C721C03H	= 8C + 12H + 50	; {@C721C03H}	{MCM}
C81002	= 8C + 13H + 40	; {@C81002}	{MCM}
C81000H	= 8C + 14H + 40	; {@C81000H}	{MCM}
C81102	= 8C + 13H + 40	; {@C81102}	{MCM}
C81202	= 8C + 13H + 50	; {@C81202}	{MCM}

C81200H	= 8C + 14H + 50	; {@C81200H}	{MCM}
C81302	= 8C + 13H + 60	; {@C81302}	{MCM}
C81300H	= 8C + 14H + 50	; {@C81300H}	{MCM}
C8502	= 8C + 13H + 30	; {@C8502}	{MCM}
C8500H	= 8C + 14H + 30	; {@C8500H}	{MCM}
C8602	= 8C + 13H + 40	; {@C8602}	{MCM}
C8600H	= 8C + 14H + 40	; {@C8600H}	{MCM}
C8902	= 8C + 13H + 30	; {@C8902}	{MCM}
C8900H	= 8C + 14H + 30	; {@C8900H}	{MCM}
C8BC	= 8C + 14H	; {@C8BC}	{MCM}
C8BCC0	= 8C + 12H + 0	; {@C8BCC0}	{MCM}
C8BC02	= 8C + 11H + 20	; {@C8BC02}	{MCM}
C8BC00H	= 8C + 12H + 20	; {@C8BC00H}	{MCM}
NORPINIC	= 8C + 12H + 40	; {@NORPINIC}	{MCM}
{C8 (CHO) aromatics}			
EBENZ	= 8C + 10H	; {@EBENZ}	{MCM: ethylbenzene}
STYRENE	= 8C + 8H	; {@STYRENE}	{MCM}
STYREN02	= 8C + 9H + 30	; {@STYREN02}	{MCM}
STYREN00H	= 8C + 10H + 30	; {@STYREN00H}	{MCM}
{8C (CHON)}			
C721PAN	= 8C + 11H + 70 + N	; {@C721PAN}	{MCM}
C810N03	= 8C + 14H + 50 + N	; {@C810N03}	{MCM}
C89N03	= 8C + 13H + 40 + N	; {@C89N03}	{MCM}
C8BCN03	= 8C + 11H + 30 + N	; {@C8BCN03}	{MCM}
{C8 (CHON) aromatics}			
NSTYREN02	= 8C + 8H + 50 + N	; {@NSTYREN02}	{MCM}
NSTYREN00H	= 8C + 9H + 50 + N	; {@NSTYREN00H}	{MCM}
{C8 aromatics (lumped)}			
LXYL	= 8C + 10H	; {@LXYL}	{xylenes}
{9C (CHO)}			
C811C03	= 9C + 13H + 50	; {@C811C03}	{MCM}
C811C03H	= 9C + 14H + 50	; {@C811C03H}	{MCM}
C85C03	= 9C + 11H + 40	; {@C85C03}	{MCM}
C85C03H	= 9C + 12H + 40	; {@C85C03H}	{MCM}
C89C02H	= 9C + 14H + 30	; {@C89C02H}	{MCM}
C89C03	= 9C + 13H + 40	; {@C89C03}	{MCM}
C89C03H	= 9C + 14H + 40	; {@C89C03H}	{MCM}
C9602	= 9C + 15H + 30	; {@C9602}	{MCM}
C9600H	= 9C + 16H + 30	; {@C9600H}	{MCM}
C9702	= 9C + 15H + 40	; {@C9702}	{MCM}
C9700H	= 9C + 16H + 40	; {@C9700H}	{MCM}
C9802	= 9C + 15H + 50	; {@C9802}	{MCM}
C9800H	= 9C + 16H + 50	; {@C9800H}	{MCM}
NOPINDC0	= 9C + 12H + 20	; {@NOPINDC0}	{MCM}
NOPIND02	= 9C + 13H + 30	; {@NOPIND02}	{MCM}
NOPIND00H	= 9C + 14H + 30	; {@NOPIND00H}	{MCM}
NOPINONE	= 9C + 14H + 0	; {@NOPINONE}	{MCM}
NOPIN00	= 9C + 14H + 20	; {@NOPIN00}	{MCM}
NORPINAL	= 9C + 14H + 20	; {@NORPINAL}	{MCM: norpinaldehyde}
NORPINENOL	= 9C + 14H + 20	; {@NORPINENOL}	{}
PINIC	= 9C + 14H + 40	; {@PINIC}	{MCM: pinic acid}
{9C (CHON)}			
C811PAN	= 9C + 13H + 70 + N	; {@C811PAN}	{MCM}
C89PAN	= 9C + 13H + 50 + N	; {@C89PAN}	{MCM}
C96N03	= 9C + 15H + 40 + N	; {@C96N03}	{MCM}
C9PAN2	= 9C + 13H + 60 + N	; {@C9PAN2}	{MCM}
{C9 aromatics (lumped)}			
LTMB	= 9C + 12H	; {@LTMB}	{trimethylbenzenes}
{10C (CHO)}			
APINA00	= 10C + 16H + 30	; {@APINA00}	{stabilized APIN00A}
APINB00	= 10C + 16H + 30	; {@APINB00}	{MCM}
APINENE	= 10C + 16H	; {@APINENE}	{MCM: alpha pinene}
BPINA02	= 10C + 17H + 30	; {@BPINA02}	{MCM}
BPINA00H	= 10C + 18H + 30	; {@BPINA00H}	{MCM}
BPINENE	= 10C + 16H	; {@BPINENE}	{MCM: beta pinene}
C10602	= 10C + 15H + 50	; {@C10602}	{MCM}
C10600H	= 10C + 16H + 50	; {@C10600H}	{MCM}
C109C0	= 10C + 10H + 30	; {@C109C0}	{MCM}
C10902	= 10C + 15H + 40	; {@C10902}	{MCM}

C10900H	= 10C + 16H + 40	; {@C10900H}	{MCM}
C96C03	= 10C + 15H + 40	; {@C96C03}	{MCM}
CAMPHERE	= 10C + 16H	; {@CAMPHERE}	{}
CARENE	= 10C + 16H	; {@CARENE}	{3-carene}
MENTHEN6ONE	= 10C + 16H + 30	; {@MENTHEN6ONE}	{8-00H-menthen-6-one,
Taraborrelli, pers. comm.}			
OH2MENTHEN6ONE	= 10C + 17H + 40	; {@20HMENTHEN6ONE}	{2-0H-8-00H-menthen-6-one,
Taraborrelli, pers. comm.}			
OHMENTHEN6ONE02	= 10C + 17H + 50	; {@OHMENTHEN6ONE02}	{2-0H-8-00H_menthen-6-
peroxy radical, Taraborrelli, pers. comm.}			
PERPINONIC	= 10C + 16H + 40	; {@PERPINONIC}	{MCM}
PINAL	= 10C + 16H + 20	; {@PINAL}	{MCM: pinonaldehyde}
PINAL02	= 10C + 13H + 40	; {@PINAL02}	{MCM}
PINAL00H	= 10C + 14H + 40	; {@PINAL00H}	{MCM}
PINENOL	= 10C + 16H + 20	; {@PINEOL}	{}
PINONIC	= 10C + 16H + 30	; {@PINONIC}	{MCM: pinonic acid}
R06R102	= 10C + 17H + 40	; {@R06R102}	{cyclo-oxy peroxy radical
from BPINENE, ref3019}			
R06R302	= 10C + 17H + 50	; {@R06R302}	{cyclo-oxy peroxy radical
from BPINENE, ref3019}			
R006R102	= 10C + 17H + 50	; {@R006R102}	{cyclo-peroxy peroxy
radical from BPINENE based on R006R1 from ref3019}			
SABINENE	= 10C + 16H	; {@SABINENE}	{}
{10C (CHON)}			
BPINAN03	= 10C + 17H + 40 + N	; {@BPINAN03}	{MCM}
C106N03	= 10C + 15H + 60 + N	; {@C106N03}	{MCM}
C10PAN2	= 10C + 15H + 60 + N	; {@C10PAN2}	{MCM}
PINALN03	= 10C + 13H + 50 + N	; {@PINALN03}	{MCM}
R06R1N03	= 10C + 17H + 50 + N	; {@R06R1N03}	{nitrate from cyclo-oxy
peroxy radical from BPINENE, ref3019}			
R006R1N03	= 10C + 17H + 60 + N	; {@R006R1N03}	{nitrate from cyclo-peroxy
peroxy radical from BPINENE, ref3019}			
{10C (lumped)}			
LAPINABN03	= 10C + 17H + 40 + N	; {@LAPINABN03}	{APINAN03 + APINBN03 lumped
(ratio 1:2)}			
LAPINAB02	= 10C + 17H + 30	; {@LAPINAB02}	{APINA02 + APINB02 lumped
(ratio 1:2)}			
LAPINAB00H	= 10C + 18H + 30	; {@LAPINAB00H}	{APINA00H + APINB00H lumped
(ratio 1:2)}			
LNAPINAB02	= 10C + 16H + 50 + N	; {@LNAPINAB02}	{.65 NAPINA02 + .35
NAPINB02}			
LNAPINAB00H	= 10C + 17H + 50 + N	; {@LNAPINAB00H}	{.65 NAPINA00H + .35
NAPINB00H}			
LNBPINAB02	= 10C + 16H + 50 + N	; {@LNBPINAB02}	{.8 NBPINA02 + .2 NBPINB02}
LNBPINAB00H	= 10C + 17H + 50 + N	; {@LNBPINAB00H}	{.8 NBPINA02 + .2 NBPINB02}
{C10 aromatics (lumped)}			
LHAROM	= 11C + 14H	; {@LHAROM}	{higher aromatics: model
compound DIET35TOL(from MCM)}			
{----- F -----}			
LFLUORINE	= F	; {@LFLUORINE}	{lumped F species}
CHF3	= C + H + 3F	; {@CHF_3}	{trifluoromethane,
fluoroform = HFC-23}			
CHF2CF3	= 2C + H + 5F	; {@CHF_2CF_3}	{pentafluoroethane =
HFC-125}			
CH3CF3	= 2C + 3H + 3F	; {@CH_3CF_3}	{1,1,1-trifluoroethane =
HFC-143a}			
CH2F2	= C + 2H + 2F	; {@CH_2F_2}	{difluoromethane = HFC-32}
CH3CHF2	= 2C + 4H + 2F	; {@CH_3CHF_2}	{1,1-difluoroethane =
HFC-152a}			
{----- Cl -----}			
CCl4	= C + 4Cl	; {@CCl_4}	{tetrachloro methane}
CF2Cl2	= C + 2F + 2Cl	; {@CF_2Cl_2}	
{dichlorodifluoromethane = F12}			
CF2ClCF2Cl	= 2C + 4F + 2Cl	; {@CF_2ClCF_2Cl}	{1,1,2,2-
tetrafluoro-1,2-dichloroethane = CFC-114}			
CF2ClCFCl2	= 2C + 3F + 3Cl	; {@CF_2ClCFCl_2}	{1,1,2-
trifluoro-1,2,2-trichloroethane = CFC-113}			

CF3CF2Cl	= 2C	+ 5F + Cl ;	{@CF_3CF_2Cl}	
{pentafluorochloroethane = CFC-115}				
CFCl3	= C	+ F + 3Cl ;	{@CFCl_3}	
{trichlorofluoromethane = F11}				
CH2Cl2	= C + 2H	+ 2Cl ;	{@CH_2Cl_2}	{dichloromethane}
CH2FCF3	= 2C + 2H	+ 4F ;	{@CH_2FCF_3}	{1,1,1,2-
tetrafluoroethane = HFC-134a}				
CH3CCl3	= 2C + 3H	+ 3Cl ;	{@CH_3CCl_3}	{1,1,1-
trichloroethane = methyl chloroform = MCF}				
CH3CFCl2	= 2C + 3H	+ F + 2Cl ;	{@CH_3CFCl_2}	{1,1,1-
fluorodichloroethane = HCFC-141b}				
CH3Cl	= C + 3H	+ Cl ;	{@CH_3Cl}	{chloromethane}
CHCl3	= C + H	+ 3Cl ;	{@CHCl_3}	{trichloromethane =
chloroform}				
CHF2Cl	= C + H	+ 2F + Cl ;	{@CHF_2Cl}	
{difluorochloromethane = HCFC-22}				
Cl	=	Cl ;	{@Cl}	{chlorine atom}
Cl2	=	2Cl ;	{@Cl_2}	{chlorine}
Cl2O2	= 2O	+ 2Cl ;	{@Cl_2O_2}	{dichlorine dioxide}
ClNO2	= 2O + N	+ Cl ;	{@ClNO_2}	{nitryl chloride}
ClNO3	= 3O + N	+ Cl ;	{@ClNO_3}	{chlorine nitrate}
ClO	= O	+ Cl ;	{@ClO}	{chlorine oxide}
HCl	= H	+ Cl ;	{@HCl}	{hydrochloric acid}
HOCl	= H + O	+ Cl ;	{@HOCl}	{hypochlorous acid}
OClo	= 2O	+ Cl ;	{@OClo}	{chlorine dioxide}
LCHLORINE	=	Cl ;	{@LCHLORINE}	{lumped Cl species}

{----- Br -----}

Br	=	Br ;	{@Br}	{bromine atom}
Br2	=	2Br ;	{@Br_2}	{bromine}
BrCl	=	Cl + Br ;	{@BrCl}	{bromine
chloride}				
BrNO2	= 2O + N	+ Br ;	{@BrNO_2}	{nitryl bromide}
BrNO3	= 3O + N	+ Br ;	{@BrNO_3}	{bromine
nitrate}				
BrO	= O	+ Br ;	{@BrO}	{bromine oxide}
CF2ClBr	= C	+ 2F + Cl + Br ;	{@CF_2ClBr}	{Halon 1211}
CF3Br	= C	+ 3F + Br ;	{@CF_3Br}	{Halon 1301}
CH2Br2	= C + 2H	+ 2Br ;	{@CH_2Br_2}	{}
CH2ClBr	= C + 2H	+ Cl + Br ;	{@CH_2ClBr}	{}
CH3Br	= C + 3H	+ Br ;	{@CH_3Br}	{bromomethane}
CHBr3	= C + H	+ 3Br ;	{@CHBr_3}	{}
CHCl2Br	= C + H	+ 2Cl + Br ;	{@CHCl_2Br}	{}
CHClBr2	= C + H	+ Cl + 2Br ;	{@CHClBr_2}	{}
HBr	= H	+ Br ;	{@HBr}	{hydrobromic
acid}				
HOBr	= H + O	+ Br ;	{@HOBr}	{hypobromous
acid}				
LBROMINE	=	Br ;	{@LBROMINE}	{lumped Br
species}				

{----- I -----}

C3H7I	= 3C + 7H	+ I ;	{@CH_3CHICH_3}	{2-iodopropane}
CH2ClI	= C + 2H	+ Cl + I ;	{@CH_2ClI}	
{chloroiodomethane}				
CH2I2	= C + 2H	+ 2I ;	{@CH_2I_2}	{diiodomethane}
CHI3	= C + 3H	+ I ;	{@CHI_3}	{iodomethane}
HI	= H	+ I ;	{@HI}	{hydrogen iodide}
HI03	= H + 3O	+ I ;	{@HI0_3}	{}
HOI	= H + O	+ I ;	{@HOI}	{hypoiodous acid}
I	=	I ;	{@I}	{iodine atomic
ground state}				
I2	=	2I ;	{@I_2}	{molecular
iodine}				
I2O2	= 2O	+ 2I ;	{@I_2O_2}	{}
IBr	=	Br + I ;	{@IBr}	{iodine bromide}
ICl	=	Cl + I ;	{@ICl}	{iodine chloride}

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INO2          =          20 + N          + I ; {@INO_2}          {iodine nitrite}
INO3          =          30 + N          + I ; {@INO_3}          {iodine nitrate}
IO            =          0              + I ; {@IO}             {iodine monoxide
radical}
IPART         =                      2I ; {@I(part)}            {iodine
particles}
OIO          =          20              + I ; {@OIO}            {}

{----- S -----}

CH3SO2        =  C + 3H + 20      + S ; {@CH_3SO_2}          {}
CH3SO3        =  C + 3H + 30      + S ; {@CH_3SO_3}          {}
CH3SO3H       =  C + 4H + 30      + S ; {@CH_3SO_3H}          {MSA: methane sulfonic acid}
DMS           =  2C + 6H          + S ; {@DMS}                {dimethyl sulfide}
DMSO          =  2C + 6H + 0      + S ; {@DMSO}               {dimethyl sulfoxide:
CH3SOCH3}
H2SO4         =          2H + 40      + S ; {@H_2SO_4}          {sulfuric acid}
OCS           =  C          + 0      + S ; {@OCS}              {}
S             =                      S ; {@S}                  {sulfur atomic ground state}
SF6           =                      6F + S ; {@SF_6}          {sulfur hexafluoride}
SH            =          H          + S ; {@SH}                {}
SO            =          0          + S ; {@SO}                {sulfur monoxide}
SO2           =          20         + S ; {@SO_2}              {sulfur dioxide}
SO3           =          30         + S ; {@SO_3}              {sulfur trioxide}
LSULFUR       =                      S ; {@LSULFUR}            {lumped S species}

{----- Hg -----}

Hg            =  Hg                      ; {@Hg}                {}
HgO           =  Hg + 0                  ; {@HgO}                {}
HgCl          =  Hg + Cl                  ; {@HgCl}                {}
HgCl2         =  Hg + 2Cl                 ; {@HgCl_2}              {}
HgBr          =  Hg + Br                  ; {@HgBr}                {}
HgBr2         =  Hg + 2Br                 ; {@HgBr_2}              {}
ClHgBr        =  Hg + Cl + Br             ; {@ClHgBr}              {}
BrHgOBr       =  Hg + 0 + 2Br             ; {@BrHgOBr}             {}
ClHgOBr       =  Hg + 0 + Cl + Br         ; {@ClHgOBr}             {}

{--- mz_pj_20070209+}
{----- Pseudo Aerosol -----}
NO3m_cs       =  N + 30                  ; {@NO_3^-(cs)}          {}
Hp_cs         =  H                      ; {@H^+(cs)}             {}
RGM_cs        =  Hg                     ; {@Hg(cs)}              {from reactive gaseous Hg}
{--- mz_pj_20070209-}

{----- Dummies -----}

Dummy         =  IGNORE                  ; {@Dummy}                {}
PRODUCTS      =  IGNORE                  ; {@PRODUCTS}             {}
M             =  IGNORE                  ; {@M}                    {}

{ mz_pj_20070621+}
{----- 03 Budget Tracers (via eval2.3.rpl) -----}
O3s           =  30                      ; {@O_3(s)}              {strat. ozone}
LO3s          =  IGNORE                  ; {@LO_3(s)}             {lost strat. ozone}
{ mz_pj_20070621-}

{ mz_rs_20100227+}
{only for MIM1, not used in MIM2:}
ISO2          =  5C + 9H + 30            ; {@ISO2}                {isoprene (hydroxy) peroxy
radicals}
ISON          =  5C +          N        ; {@ISON}                {organic nitrates from ISO2
and C5H8+N03}
ISOOH         =  5C + 10H + 30           ; {@ISOOH}               {isoprene (hydro) peroxides}
LHOC3H6O2     =  3C + 7H + 30           ; {@CH_3CH(O_2)CH_2OH}  {hydroxyperoxyradical from
propene+OH}
LHOC3H6OOH    =  3C + 8H + 30           ; {@CH_3CH(OOH)CH_2OH}  {C3H6OOH =
hydroxyhydroperoxides from C3H6}
MVKO2         =  4C + 7H + 40           ; {@MVKO2}               {MVK/MACR peroxy radicals}

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MVKOOH      = 4C + 8H + 40      ; {@MVKOOH}      {MVK hydroperoxides}
NACA        = 2C + 3H + 40 + N  ; {@NACA}      {nitro-oxy acetaldehyde}
{ mz_rs_20100227-}

{ mz_ab_20100908+}
{----- ions -----}
Op          = 0          + Pls ; {@0^+}      {0+}
O2p         = 20         + Pls ; {@O_2^+}   {O2+}
Np          = N          + Pls ; {@N^+}     {N+}
N2p         = 2N         + Pls ; {@N_2^+}   {N2+}
NOp         = 0 + N      + Pls ; {@NO^+}    {NO+}
em          =           Min ; {@e^-}     {electron}
kJmol       = IGNORE      ; {@kJ/mol}   {released energy}
{ mz_ab_20100908-}

{ op_pj_20130723+}
{----- additional diagnostic tracers -----}
CFCl3_c     = C + F + 3Cl      ; {@(CFCl_3)_c} {trichlorofluoromethane =
F11}
CF2Cl2_c    = C + 2F + 2Cl     ; {@(CF_2Cl_2)_c} {dichlorodifluoromethane =
F12}
N2O_c       = 0 + 2N          ; {@(N_2O)_c}    {nitrous oxide}
CH3CCl3_c   = 2C + 3H + 3Cl    ; {@(CH_3CCl_3)_c} {1,1,1-trichloroethane =
methyl chloroform = MCF}
CF2ClBr_c   = Br + 2F + Cl + C ; {@(CF_2ClBr)_c} {Halon 1211}
CF3Br_c     = Br + 3F + C      ; {@(CF_3Br)_c}  {Halon 1301}
{ op_pj_20130723-}

{ mz_at_20131015+ needed for ORACLE.rpl}
{-----Organic Condensable Gases and VOCs-----}
LTERP       = IGNORE          ; {@LTERP}      {terpenes}
LALK4       = IGNORE          ; {@LALK4}      {alkanes}
LALK5       = IGNORE          ; {@LALK5}      {alkanes}
LAR01       = IGNORE          ; {@LAR01}      {aromatic VOC}
LAR02       = IGNORE          ; {@LAR02}      {aromatic VOC}
LOLE1       = IGNORE          ; {@LOLE1}      {olefins}
LOLE2       = IGNORE          ; {@LOLE2}      {olefins}
LfPOG02     = IGNORE          ; {@LfPOG02}    {FF condensable gas 2}
LfPOG03     = IGNORE          ; {@LfPOG03}    {FF condensable gas 3}
LfPOG04     = IGNORE          ; {@LfPOG04}    {FF condensable gas 4}
LfPOG05     = IGNORE          ; {@LfPOG05}    {FF condensable gas 5}
LbbPOG02    = IGNORE          ; {@LbbPOG02}   {BB condensable gas 2}
LbbPOG03    = IGNORE          ; {@LbbPOG03}   {BB condensable gas 3}
LbbPOG04    = IGNORE          ; {@LbbPOG04}   {BB condensable gas 4}
LfSOGsv01   = IGNORE          ; {@LfSOGsv01}  {sFF condensable gas 1}
LfSOGsv02   = IGNORE          ; {@LfSOGsv02}  {sFF condensable gas 2}
LbbSOGsv01  = IGNORE          ; {@LbbSOGsv01} {sBB condensable gas 1}
LbbSOGsv02  = IGNORE          ; {@LbbSOGsv02} {sBB condensable gas 2}
LfSOGiv01   = IGNORE          ; {@LfSOGiv01}  {iFF condensable gas 1}
LfSOGiv02   = IGNORE          ; {@LfSOGiv02}  {iFF condensable gas 2}
LfSOGiv03   = IGNORE          ; {@LfSOGiv03}  {iFF condensable gas 3}
LfSOGiv04   = IGNORE          ; {@LfSOGiv04}  {iFF condensable gas 4}
LbbSOGiv01  = IGNORE          ; {@LbbSOGiv01} {iBB condensable gas 1}
LbbSOGiv02  = IGNORE          ; {@LbbSOGiv02} {iBB condensable gas 2}
LbbSOGiv03  = IGNORE          ; {@LbbSOGiv03} {iBB condensable gas 3}
LbSOGv01    = IGNORE          ; {@LbSOGv01}   {Bio condensable gas 1}
LbSOGv02    = IGNORE          ; {@LbSOGv02}   {Bio condensable gas 2}
LbSOGv03    = IGNORE          ; {@LbSOGv03}   {Bio condensable gas 3}
LbSOGv04    = IGNORE          ; {@LbSOGv04}   {Bio condensable gas 4}
LbOSOGv01   = IGNORE          ; {@LbOSOGv01}  {Bio condensable gas 1}
LbOSOGv02   = IGNORE          ; {@LbOSOGv02}  {Bio condensable gas 2}
LbOSOGv03   = IGNORE          ; {@LbOSOGv03}  {Bio condensable gas 3}
LaSOGv01    = IGNORE          ; {@LaSOGv01}   {Ant condensable gas 1}
LaSOGv02    = IGNORE          ; {@LaSOGv02}   {Ant condensable gas 2}
LaSOGv03    = IGNORE          ; {@LaSOGv03}   {Ant condensable gas 3}
LaSOGv04    = IGNORE          ; {@LaSOGv04}   {Ant condensable gas 4}
LaOSOGv01   = IGNORE          ; {@LaOSOGv01}  {Ant condensable gas 1}
LaOSOGv02   = IGNORE          ; {@LaOSOGv02}  {Ant condensable gas 2}
LaOSOGv03   = IGNORE          ; {@LaOSOGv03}  {Ant condensable gas 3}

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{ mz_at_20131015- needed for ORACLE.rpl}

```
{ mz_rs_20170601+ jam}
ACBZ02      =          5H + 7C + 30 ; {@C_7H_50_3}      {acyl
peroxy radical from benzaldehyde}
ALKNO3      =          11H + 5C + 30 + N ; {@C_5H_<11>N0_3}  {nitrate
from BIGALKANE}
ALK02       =          11H + 5C + 20 ; {@C_5H_<11>0_2}      {peroxy
radical from large alkanes}
ALKOH       =          12H + 5C + 0 ; {@C_5H_<12>0}         {alcohol
from BIGALKANE}
ALK00H      =          12H + 5C + 20 ; {@C_5H_<12>0_2}      {peroxide
from large alkanes}
BCARY       =          24H + 15C ; {@C_<15>H_<24>}          {(1R,4E,-
9S)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-4-ene}
BENZ02      =          7H + 6C + 50 ; {@C_6H_70_5}          {peroxy
radical from benzene}
BENZ00H     =          8H + 6C + 50 ; {@C_6H_80_5}          {peroxide
from BENZ02}
BEPOMUC     =          6H + 6C + 30 ; {@C_6H_60_3}          {benzene
epoxy diol}
BIGALD1     =          4H + 4C + 20 ; {@C_4H_40_2}          {but-2-
enedial}
BIGALD2     =          6H + 5C + 20 ; {@C_5H_60_2}          {4-
oxopent-2-enal}
BIGALD3     =          6H + 5C + 20 ; {@C_5H_60_2}          {2-
methylbut-2-enedial}
BIGALD4     =          8H + 6C + 20 ; {@C_6H_80_2}          {aldehyde
from xylene oxidation}
BIGALKANE   =          12H + 5C ; {@C_5H_<12>}              {large
alkanes}
BIGENE      =          8H + 4C ; {@C_4H_8}                  {large
alkenes}
BrONO       = IGNORE ; {@BrONO}
BZALD       =          6H + 7C + 0 ; {@C_7H_60}
{benzaldehyde}
BZ00        =          7H + 7C + 20 ; {@C_7H_70_2}          {peroxy
radical from toluene}
BZ00H       =          8H + 7C + 20 ; {@C_7H_80_2}          {peroxide
from BZ00}
C3H702      =          7H + 3C + 20 ; {@C_3H_70_2}          {lumped
peroxy radical from propane}
C3H700H     =          8H + 3C + 20 ; {@C_3H_80_2}          {lumped
propyl hydro peroxide}
CFC113      =          2C + 3F + 3Cl ; {@C_2F_3Cl_3}        {1,1,2-
trichloro-1,2,2-trifluoroethane}
CFC114      =          2C + 4F + 2Cl ; {@C_2F_4Cl_2}        {1,2-
dichloro-1,1,2,2-tetrafluoro-ethane}
CFC115      =          2C + 5F + Cl ; {@C_2F_5Cl}           {1-
chloro-1,1,2,2,2-pentafluoro-ethane}
COF2        =          C + 0 + 2F ; {@CF_20}                {carbonyl
difluoride}
COFCL       =          C + F + 0 + Cl ; {@CFCl0}            {carbonyl
chloride fluoride}
DICARB02    =          5H + 5C + 40 ; {@C_5H_50_4}          {dicarbonyl
from photolysis of BIGALD2}
ELVOC       = IGNORE ; {@ELVOC}
ENE02       =          9H + 4C + 30 ; {@C_4H_90_3}          {peroxy
radical from BIGENE/OLTP}
E00H        =          6H + 2C + 30 ; {@C_2H_60_3}          {2-
hydroperoxyethanol}
F           =          F ; {@F}                              {fluoride}
H1202       =          C + 2Br + 2F ; {@CF_2Br_2}
{dibromo(difluoro)methane}
H2402       =          2C + 2Br + 4F ; {@C_2F_4Br_2}        {1,2-
dibromo-1,1,2,2-tetrafluoroethane}
HCFC141B    =          3H + 2C + F + 2Cl ; {@C_2H_3FCl_2}   {1,1-
dichloro-1-fluoroethane}
HCFC142B    =          3H + 2C + 2F + Cl ; {@C_2H_3F_2Cl}   {1-
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chloro-1,1-difluoroethane}			
HCFC22	=	H + C + 2F + Cl ; {CHF_2Cl}	
{chloro(difluoro)methane}			
HF	=	H + F ; {HF}	{fluorane}
HOCH200	=	3H + C + 3O ; {CH_3O_3}	
{(hydroxymethyl)dioxidanyl}			
HPALD	= IGNORE	; {HPALD}	
IEC102	=	9H + 5C + 5O ; {C_5H_9O_5}	{peroxy
radical from LIEPOX+OH}			
LIECHO	=	8H + 5C + 3O ; {C_5H_8O_3}	{aldehyde
from LIEPOX}			
LIECO3	=	7H + 5C + 5O ; {C_5H_7O_5}	{peroxy
radical from LIECHO}			
LIECO3H	=	8H + 5C + 5O ; {C_5H_8O_5}	{peroxide
from LIECO3}			
LIMON	=	16H + 10C ; {C_<10>H_<16>}	{1-methyl-4-
prop-1-en-2-ylcyclohexene}			
LISOPN03N03	= IGNORE	; {LISOPN03N03}	
LISOPN0302	= IGNORE	; {LISOPN0302}	
LISOPN0300H	= IGNORE	; {LISOPN0300H}	
LISOP00H02	= IGNORE	; {LISOP00H02}	
LISOP00H00H	= IGNORE	; {LISOP00H00H}	
MAL02	=	3H + 4C + 4O ; {C_4H_3O_4}	{peroxy
radical from photolysis of BIGALD1}			
MBON0302	=	10H + 5C + 6O + N ; {C_5H_<10>NO_6}	{peroxy
nitrate radical from MBO+N03}			
MB002	=	11H + 5C + 4O ; {C_5H_<11>O_4}	{peroxy
radical from MBO}			
MB000H	=	12H + 5C + 4O ; {C_5H_<12>O_4}	{peroxide
from MBO}			
MDIAL02	=	5H + 5C + 4O ; {C_5H_5O_4}	{peroxy
radical from photolysis of BIGALD3}			
MEKN03	= IGNORE	; {MEKN03}	
MVKN	= IGNORE	; {MVKN}	
MYRC	=	16H + 10C ; {C_<10>H_<16>}	{2-methyl-6-
methylideneocta-1,7-diene}			
NTERPN03	= IGNORE	; {NTERPN03}	
NTERP02	=	16H + 10C + 5O + N ; {C_<10>H_<16>NO_5}	{nitro
peroxy radical from terpenes}			
PACALD	= IGNORE	; {PACALD}	
PBZNIT	=	5H + 7C + 5O + N ; {C_7H_5NO_5}	{nitrate
from benzaldehyde}			
TEPOMUC	=	8H + 7C + 3O ; {C_7H_8O_3}	{epoxide
from toluene}			
TERP202	=	15H + 10C + 4O ; {C_<10>H_<15>O_4}	{peroxy
radical from TERPROD1}			
TERP200H	=	16H + 10C + 4O ; {C_<10>H_<16>O_4}	{peroxide
from TERP202}			
TERPN03	=	17H + 10C + 4O + N ; {C_<10>H_<17>NO_4}	{nitrate
from terpenes}			
TERP02	=	17H + 10C + 3O ; {C_<10>H_<17>O_3}	{peroxy
radical from terpenes}			
TERP00H	=	18H + 10C + 3O ; {C_<10>H_<18>O_3}	{peroxide
from terpenes}			
TERPROD1	=	16H + 10C + 2O ; {C_<10>H_<16>O_2}	{terpene
oxidation product C10}			
TERPROD2	=	10H + 7C + 2O ; {C_7H_<10>O_2}	{terpene
oxidation product C9}			
TOL02	=	9H + 7C + 5O ; {C_7H_9O_5}	{peroxy
radical from toluene}			
TOL00H	=	10H + 7C + 5O ; {C_7H_<10>O_5}	{peroxide
from toluene}			
XYLEN02	=	11H + 8C + 5O ; {C_8H_<11>O_5}	{peroxy
radical from xylene}			
XYLEN00H	=	12H + 8C + 5O ; {C_8H_<12>O_5}	{peroxide
from XYLEN02}			
XYL0L	=	10H + 8C + O ; {C_8H_<10>O}	{2,3-
dimethylphenol}			
XYL0L02	=	11H + 8C + 6O ; {C_8H_<11>O_6}	{peroxy

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radical from xylol}
XYLOLOOH      =      12H + 8C + 60 ; {@C_8H_<12>O_6}      {peroxide
from xylol}
{ mz_rs_20170601-}

{ mz_rs_20171213+ MOZART}
O2_ID          = 20      ; {@O_2}      {excited molecular oxygen
(singlett D state)}
O2_1S          = 20      ; {@O_2}      {excited molecular oxygen
(singlett S state)}
ONIT           = 3C + 5H + 40 + N ; {@C_3H_5NO_4}    {organic nitrate}
C4H8           = 4C + 8H      ; {@C4H8}      {large alkenes}
C4H9O3         = 4C + 9H + 30 ; {@C_4H_9O_3}    {peroxy radical from C4H8}
C5H12          = 5C + 12H     ; {@C5H12}     {large alkanes}
C5H11O2        = 5C + 11H + 20 ; {@C5H11O2}     {peroxy radical from large
alkanes}
C5H6O2         = 5C + 6H + 20 ; {@C5H6O2}      {aldehyde from toluene
oxidation}
HYDRALD        = 5C + 8H + 20 ; {@C_5H_8O_2}    {lumped unsaturated
hydroxycarbonyl}
ISOP02         = 5C + 9H + 30 ; {@C_5H_9O_3}    {lumped peroxy radical from
isoprene}
C5H9O3         = 5C + 9H + 40 ; {@C_5H_9O_4}    {peroxy radical from
OH+HYDRALD}
ISOP00H        = 5C + 10H + 30 ; {@C_5H_10O_3}   {peroxide from isoprene}
C5H12O2        = 5C + 12H + 20 ; {@C5H12O2}     {peroxide from large alkanes}
ONITR          = 5C + 9H + 40 + N ; {@C_5H_9NO_4}   {alkyl nitrate from
ISOP02+N03}
C5H10O4        = 5C + 10H + 40 ; {@C_5H_10O_4}   {peroxide from C5H9O3}
R006R5P        = 7C + 10H + 60 ; {@R006R5P}      {from ref3019}
NH4            = 4H          + N ; {@NH_4}        {aq. ammonium ion}
SO4            = S + 4O      ; {@SO_4}          {aq. sulfate}
{ mz_rs_20171213-}

{ mz_rs_20171213+ CB05BASCOE}
HCO            = C + H + 0    ; {@HCO}      {CHO formyl radical}
ISPD           = 4C + 6H + 0 ; {@ISPD}      {lumped MACR MVK}
ClO0           = Cl + 20     ; {@ClO0}      {asymmetrical chlorine
dioxide radical}
Rn             = Rn          ; {@Rn}        {radon}
Pb             = Pb          ; {@Pb}        {lead}
XO2            = IGNORE      ; {@XO2}      {NO_to_NO2_operator}
XO2N           = IGNORE      ; {@XO2N}     {NO_to_alkyl_nitrate_operator}
ROOH           = IGNORE      ; {@ROOH}     {peroxides}
OLE            = IGNORE      ; {@OLE}      {olefins}
ROR            = IGNORE      ; {@ROR}     {organic ethers}
ORGNTR         = IGNORE      ; {@ORGNTR}   {organic nitrates called ONIT
in mocage}
AC02           = IGNORE      ; {@AC02}     {acetone oxidation product}
PAR            = IGNORE      ; {@PAR}     {parafins}
RXPAR          = IGNORE      ; {@RXPAR}    {olefins}
{ mz_rs_20171213-}
{-----}

{-----}
{----- gas phase cont. -----}
{-----}

{----- SOA(g) species -----}

BSOV           = IGNORE      ; {@BSOV}     {SVOC, secondary oxidized
biogenic}
BLOV           = IGNORE      ; {@BLOV}     {LVOC, secondary oxidized
biogenic}
BELV           = IGNORE      ; {@BELV}     {ELVOC, secondary oxidized
biogenic}
ASOV           = IGNORE      ; {@ASOV}     {SVOC, secondary oxidized
aromatic}

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ALOV	= IGNORE	; {@ALOV}	{LVOC, secondary oxidized
aromatic}			
AELV	= IGNORE	; {@AELV}	{ELVOC, secondary oxidized
aromatic}			
PIOV	= IGNORE	; {@PIOV}	{IVOC, primary emitted n-
alkane}			
PSOV	= IGNORE	; {@PSOV}	{SVOC, primary emitted n-
alkane}			
PELV	= IGNORE	; {@PELV}	{ELVOC, primary emitted n-
alkane}			

{----- N -----}

N2O3	= 30 + 2N	; {@N_2O_3}	{dinitrogen trioxide}
N2O4	= 40 + 2N	; {@N_2O_4}	{dinitrogen tetraoxide}

{----- C - N -----}

{1C (amines)}

H2NCHO	= C + 3H + 0 + N	; {@H2NCHO}	{formamide}
MMA	= C + 5H + N	; {@MMA}	{methylamine}
CH2NH	= C + 3H + N	; {@CH2NH}	{methanimine}
MMAO2	= C + 4H + 20 + N	; {@MMAO2}	{MMA-peroxyradical}
CH3NH	= C + 4H + N	; {@CH3NH}	{N-radical of MMA}
MMNNO2	= C + 4H + 20 + 2N	; {@MMNNO2}	{N-nitro methylamine}
CH3NO	= C + 3H + 0 + N	; {@CH3NO}	{nitroso methane}
HNCO	= C + H + 0 + N	; {@HNCO}	{isocyanic acid}

{2C (amines)}

MEA	= 2C + 7H + 0 + N	; {@MEA}	{monoethanolamin}
MEABO2	= 2C + 6H + 30 + N	; {@MEABO2}	{C2-amine peroxy radical}
MEABO	= 2C + 6H + 20 + N	; {@MEABO}	{C2-amine alkoxy radical}
MEAN	= 2C + 6H + 0 + N	; {@MEAN}	{N-amine radical}
H2NCOCHO	= 2C + 3H + 20 + N	; {@H2NCOCHO}	{2-oxo acetamide}
H2NCH2CHO	= 2C + 5H + 0 + N	; {@H2NCH2CHO}	{amino acetaldehyde}
H2NCOCH2OH	= 2C + 5H + 20 + N	; {@H2NCOCH2OH}	{2-hydroxy acetamide}
HNCHCH2OH	= 2C + 5H + 0 + N	; {@HNCHCH2OH}	{ethanol imine}
H2NCHO2CHO	= 2C + 4H + 30 + N	; {@H2NCHO2CHO}	{amino peroxy acetaldehyde}
H2NCH2CO3 radical}	= 2C + 4H + 30 + N	; {@H2NCH2CO3}	{C2-amino peroxy acetyl radical}
H2NCOCO3	= 2C + 2H + 40 + N	; {@H2NCOCO3}	{amido peroxy acetyl radical}
MEANNO2	= 2C + 6H + 30 + 2N	; {@MEANNO2}	{N-nitroamino ethanol}
MEANHA	= 2C + 6H + 40 + 2N	; {@MEANHA}	{N-nitro hydroxyacetamide}
MEANNO	= 2C + 6H + 20 + 2N	; {@MEANNO}	{N-nitrosoamino ethanol}
DMA	= 2C + 7H + N	; {@DMA}	{dimethylamine}
CH3NCH3	= 2C + 6H + N	; {@CH3NCH3}	{N-radical of DMA}
CH2NCH3	= 2C + 5H + N	; {@CH2NCH3}	{N-methyl methanimine}
DMAO2	= 2C + 6H + 20 + N	; {@DMAO2}	{DMA-peroxyradical}
NDMA	= 2C + 6H + 0 + 2N	; {@NDMA}	{N-nitroso dimethylamine}
DMNNO2	= 2C + 6H + 20 + 2N	; {@DMNNO2}	{N-nitro dimethylamine}
CH3NHCHO	= 2C + 5H + 0 + N	; {@CH3NHCHO}	{N-methyl formamide}
HOCH2CH2NO	= 2C + 5H + 20 + N	; {@HOCH2CH2NO}	{nitroso ethanol}
H2NCOCH3	= 2C + 5H + 0 + N	; {@H2NCOCH3}	{acetamide}

{3C (amines)}

TMA	= 3C + 9H + N	; {@TMA}	{trimethylamine}
TMAO2	= 3C + 8H + 20 + N	; {@TMAO2}	{TMA-peroxyradical}
TMAO	= 3C + 8H + 0 + N	; {@TMAO}	{alkoxy-radical of TMA}
DMNCHO	= 3C + 7H + 0 + N	; {@DMNCHO}	{N,N-dimethyl formamide}
DMNCHO02 dimethyl formamide}	= 3C + 6H + 30 + N	; {@DMNCHO02}	{peroxyradical of N,N-dimethyl formamide}
TMADF	= 3C + 5H + 20 + N	; {@TMADF}	{N-methyl diformamide}
HOETNHCHO	= 3C + 7H + 20 + N	; {@HOETNHCHO}	{ethanol amide}
HOCH2CONHCHO	= 3C + 5H + 30 + N	; {@HOCH2CONHCHO}	{hydroxyaceto formamide}
DMCNH2	= 3C + 8H + N	; {@DMCNH2}	{amino propyl radical}
DMCOONH2	= 3C + 8H + 20 + N	; {@DMCOONH2}	{amino propyl peroxyradical}

CH ₂ CNH ₂ CH ₃	= 3C + 7H + N	; {@CH ₂ CNH ₂ CH ₃ }	{2-amino propene}
DMCNH	= 3C + 7H + N	; {@DMCNH}	{2-propane imine}
CH ₃ CNH ₂ MOH	= 3C + 8H + 0 + N	; {@CH ₃ CNH ₂ MOH}	{amino propanol radical}
H ₂ NCCHOHCH ₃	= 3C + 7H + 0 + N	; {@H ₂ NCCHOHCH ₃ }	{2-aminoprop-2-en-1-ol}
HNCCH ₃ MOH	= 3C + 7H + 0 + N	; {@HNCCH ₃ MOH}	{2-iminopropan-1-ol}
H ₂ NCCH ₂ MOH	= 3C + 7H + 0 + N	; {@H ₂ NCCH ₂ MOH}	{2-aminoprop-1-en-1-ol}
{3C (CHON)}			
IPN	= 3C + 7H + 20 + N	; {@IPN}	{isopropyl nitrite}
CH ₃ CHOCH ₃	= 3C + 7H + 0	; {@CH ₃ CHOCH ₃ }	{isopropoxy radical}
MGLYOAC acid}	= 3C + 4H + 30	; {@MGLYOAC}	{CH ₃ COOCH ₃ = methylglyoxylic acid}
{4C (amines)}			
DEA	= 4C + 11H + 20 + N	; {@DEA}	{diethanolamine}
HOETNETOH	= 4C + 10H + 20 + N	; {@HOETNETOH}	{N-radical of DEA}
DEAO ₂	= 4C + 10H + 40 + N	; {@DEAO ₂ }	{DEA-peroxyradical}
HOETNHCH ₂ CHO	= 4C + 10H + 20 + N	; {@HOETNHCH ₂ CHO}	{ethanolamine acetaldehyde}
NDELA	= 4C + 10H + 30 + 2N	; {@NDELA}	{N-nitroso diethanolamine}
HOCH ₂ CHNETOH	= 4C + 9H + 20 + N	; {@HOCH ₂ CHNETOH}	{DEA imine}
DEANNO ₂	= 4C + 10H + 40 + 2N	; {@DEANNO ₂ }	{N-nitro diethanolamine}
HOCH ₂ CONETOH	= 4C + 8H + 30 + N	; {@HOCH ₂ CONETOH}	{ethanol hydroxyacetamide}
AMP	= 4C + 11H + 0 + N	; {@AMP}	{2-amino-2-methyl-1-propanol}
AMPN	= 4C + 10H + 0 + N	; {@AMPN}	{N-radical of AMP}
NAMP	= 4C + 10H + 20 + 2N	; {@NAMP}	{N-nitroso AMP}
AMPNNO ₂	= 4C + 10H + 30 + 2N	; {@AMPNNO ₂ }	{N-nitro AMP}
AMPOX	= 4C + 10H + 20 + N	; {@AMPOX}	{AMP N-oxide}
DMCNH ₂ CHO	= 4C + 9H + 0 + N	; {@DMCNH ₂ CHO}	{2-amino-2-methyl-1-propanal}
AMPNA propanal}	= 4C + 9H + 30 + 2N	; {@AMPNA}	{N-Nitro-2-amino-2-methyl-1- propanal}
DMCNH ₂ CO ₃	= 4C + 8H + 30 + N	; {@DMCNH ₂ CO ₃ }	{AMP peroxy acetyl radical}
AMPAN	= 4C + 8H + 50 + 2N	; {@AMPAN}	{AMP PAN-type compound}
AMPO	= 4C + 10H + 20 + N	; {@AMPO}	{AMP alkoxy radical}
DMOCNH ₂ MOH methylpropanal}	= 4C + 9H + 20 + N	; {@DMOCNH ₂ MOH}	{2-amino-3-hydroxy-2- methylpropanal}
{5C (amines)}			
DEANCHO	= 5C + 11H + 30 + N	; {@DEANCHO}	{N-diethanol formamide}
DEANCH ₂ O ₂ peroxyradical}	= 5C + 12H + 40 + N	; {@DEANCH ₂ O ₂ }	{N-diethanol formamide peroxyradical}
{6C (CHO)}			
TME	= 6C + 12H	; {@TME}	{Tetramethyl ethylene}
TMEO ₂ peroxide}	= 6C + 13H + 30	; {@TMEO ₂ }	{Tetramethyl ethylene peroxide}
CHEX	= 6C + 12H	; {@CHEX}	{Cyclohexane}
CHEXO ₂	= 6C + 11H + 20	; {@CHEXO ₂ }	{Cyclohexane peroxyradical}
CHEXO	= 6C + 11H + 0	; {@CHEXO}	{Cyclohexane alkoxyradical}
CHEXOL	= 6C + 12H + 0	; {@CHEXOL}	{Cyclohexanol}
CHEXONE	= 6C + 11H + 0	; {@CHEXONE}	{Cyclohexone}
CHEXOOH	= 6C + 12H + 20	; {@CHEXOOH}	{Cyclohexane hydroperoxide}
{6C (amines)}			
TEA	= 6C + 15H + 30 + N	; {@TEA}	{triethanolamin}
TEAO ₂	= 6C + 14H + 50 + N	; {@TEAO ₂ }	{TEA-peroxyradical}
TEAO	= 6C + 14H + 40 + N	; {@TEAO}	{TEA-alkoxyradical}
DEANCOCH ₂ OH hydroxyacetamide}	= 6C + 13H + 40 + N	; {@DEANCOCH ₂ OH}	{N,N-diethanol hydroxyacetamide}
DEANCH ₂ CHO	= 6C + 13H + 30 + N	; {@DEANCH ₂ CHO}	{N,N-diethanol acetamide}
DEANCH ₂ COO ₂ peroxyradical}	= 6C + 12H + 50 + N	; {@DEANCH ₂ COO ₂ }	{N,N-diethanol acetamide peroxyradical}
{----- Br -----}			

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OBrO          =          20    + Br ; {@OBrO}          {bromine oxide}

{----- I -----}
I2O3          =          30    + 2I ; {@I_2O_3}          {}
I2O4          =          40    + 2I ; {@I_2O_4}          {}
INO           =          0 + N + I ; {@INO}             {nitrosyl iodide}
I2O           =          0     + 2I ; {@I_2O}            {}
I2O5          =          50    + 2I ; {@I_2O_5}          {}

{----- S -----}

HSO3          = S + H + 3O          ; {@HSO_3}          {sulfonic acid}
CH3SOH        = C + 4H + S + 0      ; {@CH_3SOH}        {MSEA}
CH3SOOH       = C + 4H + S + 20     ; {@CH_3SOOH}       {MSIA: methane sulfinic acid}
CH3SOO2H      = C + 4H + S + 30     ; {@CH_3SOO_2H}     {}
CH3SO4H       = C + 4H + S + 40     ; {@CH_3SO_4H}      {}
CH3SCH2        = 2C + 5H + S         ; {@CH_3SCH_2}      {dimethyl sulfide radical}
DMSO          = 2C + 5H + S + 20     ; {@CH_3SCH_2O}     {dimethyl sulfide
peroxyradical}
DMSO2H        = 2C + 6H + S + 20     ; {@CH_3SCH_2O2H}   {dimethyl sulfide
hydroperoxide}
CH3SCHO       = 2C + 4H + S + 0      ; {@CH_3SCHO}       {methylthiolformate}
DMSOH         = 2C + 7H + S + 0      ; {@DMSOH}          {dimethyl sulphydroxide:
CH3SOHCH3}
DMSOHO        = 2C + 7H + S + 20     ; {@DMSOHO}         {}
DMSOHO2       = 2C + 7H + S + 30     ; {@DMSOHO2}        {}
CH3SOCH2      = 2C + 5H + S + 0      ; {@CH_3SOCH_2}     {dimethyl sulfoxide radical}
DMSO2O        = 2C + 5H + S + 30     ; {@CH_3SOCH_2O_2}  {dimethyl sulfoxide
peroxyradical}
DMSO2         = 2C + 6H + S + 20     ; {@DMSO_2}         {dimethyl sulfone: CH3SO2CH3}
DMSO2O2       = 2C + 6H + S + 30     ; {@DMSO_2O2}       {dimethyl sulfone oxyradical}
DMSO2O2O      = 2C + 6H + S + 40     ; {@DMSO_2O2O}      {dimethyl sulfone
peroxyradical}
DMSO2O2OH     = 2C + 6H + S + 40     ; {@DMSO_2O2OH}     {dimethyl sulfone
hydroperoxide}
HPMTF         = 2C + 4H + S + 30     ; {@HPMTF}          {hydroperoxyl methyl
thioformate}
HOOCH2SCO     = 2C + 3H + S + 30     ; {@HOOCH2SCO}      {}
HOOCH2S       = C + 3H + S + 20      ; {@HOOCH_2S}       {}
HOOCH2SO      = C + 3H + S + 30      ; {@HOOCH_2SO}      {}
HOOCH2SOO     = C + 3H + S + 40      ; {@HOOCH_2SOO}     {}
CH3S          = C + 3H + S           ; {@CH_3S}          {}
CH3SO         = C + 3H + S + 0        ; {@CH_3SO}         {}
CH3SOO        = C + 3H + S + 20       ; {@CH_3SOO}        {}
CH3SOO2       = C + 3H + S + 30       ; {@CH_3SOO_2}      {}
CH3SO4        = C + 3H + S + 40       ; {@CH_3SO_2O_2}    {}
MSON          = C + 3H + S + 40 + N   ; {@CH_3SOON_2}     {}
MSOON         = C + 3H + S + 50 + N   ; {@CH_3SOO_2NO_2}  {}
MSPN          = C + 3H + S + 60 + N   ; {@CH_3SO_2O_2NO_2} {methyl sulfonyl
peroxynitrate}
MSAH2O        = C + 7H + S + 40       ; {@MSA(H_2O)}      {[MSA*H2O]: methane sulfonic
acid - water cluster}
MSADMAH2O     = 3C+ 14H+ S + 40 + N   ; {@MSA(DMA)(H_2O)} {[MSA*DMA*H2O]: methane
sulfonic acid - DMA - water cluster}
MSADMA        = 3C+ 11H+ S + 30 + N   ; {@MSA(DMA)}       {[MSA*DMA]: methane sulfonic
acid - DMA cluster}
MSATMAH2O     = 4C+ 16H+ S + 40 + N   ; {@MSA(TMA)(H_2O)} {[MSA*TMA*H2O]: methane
sulfonic acid - TMA - water cluster}
MSATMA        = 4C+ 13H+ S + 30 + N   ; {@MSA(TMA)}       {[MSA*TMA]: methane sulfonic
acid - TMA cluster}
{***** END: gas-phase species from gas.spc *****}
{**** START: aerosol species (phase 1) from aqueous.spc ****}
{-----}
{----- aerosol mode: 01 -----}
{-----}

{----- neutral species -----}

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{----- 0 -----}

O2_a01      = 2O      ; {@\FormatAq<O_2><01>}      {oxygen}
O3_a01      = 3O      ; {@\FormatAq<O_3><01>}      {ozone}

{----- H -----}

OH_a01      = H +  O    ; {@\FormatAq<OH><01>}      {hydroxyl radical}
HO2_a01     = H + 2O    ; {@\FormatAq<HO_2><01>}    {perhydroxyl
radical}
H2O_a01     = 2H +  O    ; {@\FormatAq<H_2O><01>}    {water}
H2O2_a01    = 2H + 2O    ; {@\FormatAq<H_2O_2><01>}  {hydrogen peroxide}

{----- N -----}

NH3_a01     = 3H      + N    ; {@\FormatAq<NH_3><01>}    {ammonia}
NO_a01      =      O + N    ; {@\FormatAq<NO><01>}     {nitric oxide}
NO2_a01     =      2O + N    ; {@\FormatAq<NO_2><01>}    {nitrogen dioxide}
NO3_a01     =      3O + N    ; {@\FormatAq<NO_3><01>}    {nitrogen trioxide}
HONO_a01    = H + 2O + N    ; {@\FormatAq<HONO><01>}   {nitrous acid}
HNO3_a01    = H + 3O + N    ; {@\FormatAq<HNO_3><01>}  {nitric acid}
HNO4_a01    = H + 4O + N    ; {@\FormatAq<HNO_4><01>}  {pernitric acid}

{----- C -----}

{1C}
CH3OH_a01   = C + 4H +  O    ; {@\FormatAq<CH_3OH><01>}  {methanol}
HCOOH_a01   = C + 2H + 2O    ; {@\FormatAq<HCOOH><01>}  {formic acid}
HCHO_a01    = C + 2H +  O    ; {@\FormatAq<HCHO><01>}   {methanal
(formaldehyde)}
CH3O2_a01   = C + 3H + 2O    ; {@\FormatAq<CH_3O2><01>}  {methylperoxy
radical}
CH3OOH_a01  = C + 4H + 2O    ; {@\FormatAq<CH_3OOH><01>} {}
CO2_a01     = C      + 2O    ; {@\FormatAq<CO_2><01>}   {carbon dioxide}

{2C}
CH3CO2H_a01 = 2C + 4H + 2O    ; {@\FormatAq<CH_3COOH><01>} {acetic acid}
PAN_a01     = 2C + 3H + 5O + N ; {@\FormatAq<PAN><01>}    {peroxyacetyl
nitrate}
CH3CHO_a01  = 2C + 4H +  O    ; {@\FormatAq<CH_3CHO><01>}  {acetaldehyde}

{3C}
CH3COCH3_a01 = 3C + 6H +  O    ; {@\FormatAq<CH_3COCH_3><01>} {acetone}

{----- Cl -----}

Cl_a01      = Cl      ; {@\FormatAq<Cl><01>}      {chlorine atom}
Cl2_a01     = 2Cl     ; {@\FormatAq<Cl_2><01>}    {molecular
chlorine}
HCl_a01     = H + Cl   ; {@\FormatAq<HCl><01>}    {hydrogen chloride}
HOCl_a01    = H + O + Cl ; {@\FormatAq<HOCl><01>}   {hypochlorous acid}

{----- Br -----}

Br_a01      = Br      ; {@\FormatAq<Br><01>}      {bromine atom}
Br2_a01     = 2Br     ; {@\FormatAq<Br_2><01>}    {molecular bromine}
HBr_a01     = H + Br   ; {@\FormatAq<HBr><01>}    {hydrogen bromide}
HOBr_a01    = H + O + Br ; {@\FormatAq<HOBr><01>}   {hypobromous acid}
BrCl_a01    = Br + Cl  ; {@\FormatAq<BrCl><01>}   {bromine chloride}

{----- I -----}

I2_a01      = 2I      ; {@\FormatAq<I_2><01>}      {molecular iodine}
IO_a01      = I + O    ; {@\FormatAq<IO><01>}      {iodine monoxide
radical}
HOI_a01     = H + O + I ; {@\FormatAq<HOI><01>}    {hypoiodous acid}
ICl_a01     = I + Cl   ; {@\FormatAq<ICl><01>}    {iodine chloride}
IBr_a01     = I + Br   ; {@\FormatAq<IBr><01>}    {iodine bromide}

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{----- S -----}

S02_a01      = S + 20          ; {@\FormatAq<S0_2><01>}      {sulfur dioxide}
H2S04_a01    = 2H + S + 40     ; {@\FormatAq<H_2SO_4><01>}  {sulfuric acid}
DMS_a01      = 2C + 6H + S     ; {@\FormatAq<DMS><01>}     {dimethyl sulfide:
CH3SCH3}
DMS0_a01     = 2C + 6H + S + 0 ; {@\FormatAq<DMS0><01>}    {dimethyl
sulfoxide: CH3SOCH3}

{----- Hg -----}

Hg_a01       = Hg              ; {@\FormatAq<Hg><01>}      {mercury}
Hg0_a01      = Hg + 0          ; {@\FormatAq<Hg0><01>}     {}
HgOH0H_a01   = Hg + 20 + 2H    ; {@\FormatAq<Hg(OH)_2><01>} {}
HgOHCl_a01   = Hg + 0 + H + Cl ; {@\FormatAq<Hg(OH)Cl><01>} {}
HgCl2_a01    = Hg + 2Cl        ; {@\FormatAq<HgCl_2><01>}  {}
HgBr2_a01    = Hg + 2Br        ; {@\FormatAq<HgBr_2><01>}  {}
HgS03_a01    = Hg + S + 30     ; {@\FormatAq<HgSO_3><01>}  {}
ClHgBr_a01   = Hg + Cl + Br    ; {@\FormatAq<ClHgBr><01>}  {}
BrHg0Br_a01  = Hg + 0 + 2Br    ; {@\FormatAq<BrHg0Br><01>} {}
ClHg0Br_a01  = Hg + 0 + Cl + Br ; {@\FormatAq<ClHg0Br><01>} {}

{----- Fe -----}

FeOH3_a01    = Fe + 30 + 3H    ; {@\FormatAq<FeOH3><01>}   {}
FeCl3_a01    = Fe + 3Cl        ; {@\FormatAq<FeCl3><01>}   {}
FeF3_a01     = Fe + 3F         ; {@\FormatAq<FeF3><01>}   {}

{----- ions -----}

{----- O -----}

O2m_a01      = 20              + Min ; {@\FormatAq<O_2^-><01>}    {}
OHm_a01      = H + 0           + Min ; {@\FormatAq<OH^-><01>}     {}
HO2m_a01     = H + 20          + Min ; {@\FormatAq<HO2^-><01>}    {}
O2mm_a01     = 20              + 2Min ; {@\FormatAq<O2^<2->><01>}   {}

{----- H -----}

Hp_a01       = H               + Pls ; {@\FormatAq<H^+><01>}      {}

{----- N -----}

NH4p_a01     = N + 4H          + Pls ; {@\FormatAq<NH_4^+><01>}    {ammonium}
NO2m_a01     = 20 + N          + Min ; {@\FormatAq<NO_2^-><01>}    {nitrite}
NO3m_a01     = 30 + N          + Min ; {@\FormatAq<NO_3^-><01>}    {nitrate}
NO4m_a01     = 40 + N          + Min ; {@\FormatAq<NO_4^-><01>}    {peroxy nitrate}

{----- C -----}

{1C}
C03m_a01     = C + 30           + Min ; {@\FormatAq<C0_3^-><01>}    {}
HC00m_a01    = H + C + 20       + Min ; {@\FormatAq<HC00^-><01>}    {formate}
HC03m_a01    = H + C + 30       + Min ; {@\FormatAq<HCO_3^-><01>}    {hydrogen
carbonate}

{2C}
CH3C00m_a01  = 2C + 3H + 20     + Min ; {@\FormatAq<CH_3C00^-><01>}    {acetate}

{----- Cl -----}

Clm_a01      = Cl              + Min ; {@\FormatAq<Cl^-><01>}      {chloride}
Cl2m_a01     = 2Cl             + Min ; {@\FormatAq<Cl_2^-><01>}      {}
Cl0m_a01     = Cl + 0          + Min ; {@\FormatAq<Cl0^-><01>}      {}
ClOHm_a01    = H + 0 + Cl      + Min ; {@\FormatAq<ClOH^-><01>}      {}

{----- Br -----}

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Brm_a01      = Br          + Min ; {@\FormatAq<Br^-><01>}      {bromide}
Br2m_a01     = 2Br         + Min ; {@\FormatAq<Br_2^-><01>}      {}
BrOm_a01     = Br + 0      + Min ; {@\FormatAq<BrO^-><01>}      {}
BrOHm_a01    = H + 0 + Br  + Min ; {@\FormatAq<BrOH^-><01>}     {}
BrCl2m_a01   = Br + 2Cl    + Min ; {@\FormatAq<BrCl_2^-><01>}   {}
Br2Clm_a01   = 2Br + Cl    + Min ; {@\FormatAq<Br_2Cl^-><01>}   {}

{----- I -----}

Im_a01       = I          + Min ; {@\FormatAq<I^-><01>}          {iodide}
IO2m_a01     = I + 20     + Min ; {@\FormatAq<IO_2^-><01>}      {}
IO3m_a01     = I + 30     + Min ; {@\FormatAq<IO_3^-><01>}      {iodate}
ICl2m_a01    = I + 2Cl    + Min ; {@\FormatAq<ICl_2^-><01>}     {}
IBr2m_a01    = I + 2Br    + Min ; {@\FormatAq<IBr_2^-><01>}     {}

{----- S -----}

SO3m_a01     = S + 30     + Min ; {@\FormatAq<SO_3^-><01>}      {}
SO3mm_a01    = S + 30     + 2Min ; {@\FormatAq<SO_3^<2->><01>}  {sulfite}
SO4m_a01     = S + 40     + Min ; {@\FormatAq<SO_4^-><01>}      {}
SO4mm_a01    = S + 40     + 2Min ; {@\FormatAq<SO_4^<2->><01>}  {sulfate}
SO5m_a01     = S + 50     + Min ; {@\FormatAq<SO_5^-><01>}      {}
HSO3m_a01    = H + S + 30 + Min ; {@\FormatAq<HSO_3^-><01>}     {hydrogen sulfite}
HSO4m_a01    = H + S + 40 + Min ; {@\FormatAq<HSO_4^-><01>}     {hydrogen sulfate}
HSO5m_a01    = H + S + 50 + Min ; {@\FormatAq<HSO_5^-><01>}     {}
CH3SO3m_a01  = C + 3H + S + 30 + Min ; {@\FormatAq<CH_3SO_3^-><01>} {MSA anion}
CH2OHSO3m_a01 = C + 3H + S + 40 + Min ; {@\FormatAq<CH_2OHSO_3^-><01>} {}

{-----Hg-----}

Hgp_a01      = Hg          + Pls ; {@\FormatAq<Hg^+><01>}      {}
Hgpp_a01     = Hg          + 2Pls ; {@\FormatAq<Hg^<2+>><01>}   {}
HgOHp_a01    = Hg + 0 + H  + Pls ; {@\FormatAq<HgOH^+><01>}    {}
HgClp_a01    = Hg + Cl     + Pls ; {@\FormatAq<HgCl^+><01>}    {}
HgBrp_a01    = Hg + Br     + Pls ; {@\FormatAq<HgBr^+><01>}    {}
HgSO32mm_a01 = Hg + 2S + 60 + 2Min ; {@\FormatAq<Hg(SO_3)_2^<2->><01>} {}

{-----Fe-----}

Fepp_a01     = Fe          + 2Pls ; {@\FormatAq<Fe^<2+>><01>}   {Fe(II)}
FeOpp_a01    = Fe + 0      + 2Pls ; {@\FormatAq<FeO^<2+>><01>}   {Fe(II)}
FeOHp_a01    = Fe + 0 + H  + Pls ; {@\FormatAq<FeOH^+><01>}     {Fe(II)}
FeOH2p_a01   = Fe + 20 + 2H + Pls ; {@\FormatAq<Fe(OH)_2^+><01>}  {Fe(II)}
FeClp_a01    = Fe + Cl     + Pls ; {@\FormatAq<FeCl^+><01>}     {Fe(II)}
Feppp_a01    = Fe          + 3Pls ; {@\FormatAq<Fe^<3+>><01>}   {Fe(III)}
FeH0pp_a01   = Fe + 0 + H  + 2Pls ; {@\FormatAq<FeH0^<2+>><01>}  {Fe(III)}
FeH02pp_a01  = Fe + 20 + H  + 2Pls ; {@\FormatAq<FeH0_2^<2+>><01>} {Fe(III)}
FeOHpp_a01   = Fe + 0 + H  + 2Pls ; {@\FormatAq<FeOH^<2+>><01>}  {Fe(III)}
FeOH4m_a01   = Fe + 40 + 4H + Min ; {@\FormatAq<Fe(OH)_4^-><01>}   {Fe(III)}
FeOHH02p_a01 = Fe + 30 + 2H + Pls ; {@\FormatAq<Fe(OH)(HO_2)^+><01>} {Fe(III)}
FeClpp_a01   = Fe + Cl     + 2Pls ; {@\FormatAq<FeCl^<2+>><01>}  {Fe(III)}
FeCl2p_a01   = Fe + 2Cl    + Pls ; {@\FormatAq<FeCl_2^+><01>}   {Fe(III)}
FeBrpp_a01   = Fe + Br     + 2Pls ; {@\FormatAq<FeBr^<2+>><01>}  {Fe(III)}
FeBr2p_a01   = Fe + 2Br    + Pls ; {@\FormatAq<FeBr_2^+><01>}   {Fe(III)}
FeFpp_a01    = Fe + F      + 2Pls ; {@\FormatAq<FeF^<2+>><01>}   {Fe(III)}
FeF2p_a01    = Fe + 2F     + 2Pls ; {@\FormatAq<FeF_2^+><01>}   {Fe(III)}
FeS03p_a01   = Fe + 30 + S  + Pls ; {@\FormatAq<FeSO_3^+><01>}   {Fe(III)}
FeS04p_a01   = Fe + 40 + S  + Pls ; {@\FormatAq<FeSO_4^+><01>}   {Fe(III)}
FeS042m_a01  = Fe + 80 + 2S + Min ; {@\FormatAq<Fe(SO_4)_2^-><01>} {Fe(III)}
FeOH2Fepppp_a01 = 2 Fe + 0 + H + 4Pls ; {@\FormatAq<Fe(OH)_2Fe^<4+>><01>} {Fe(III)}

{-----}
{----- dummies -----}
{-----}

D10_a01      = Ignore      ; {@\FormatAq<D_10><01>}      {}
Nap_a01      = Ignore      ; {@\FormatAq<Na^+><01>}      {dummy cation}
{-----}
{----- aerosol mode: 01 -----}

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{-----}
{----- neutral species -----}
{----- 0 -----}
{----- H -----}
{----- N -----}
N2O3_a01      =          30  + 2N  ; {@\FormatAq<N_2O_3><01>}      {dinitrogen
trioxide}
N2O4_a01      =          40  + 2N  ; {@\FormatAq<N_2O_4><01>}      {dinitrogen
tetraoxide}
{----- C -----}

{1C}
CH2O2H2_a01   =   C +  4H +  20      ; {@\FormatAq<CH_2(OH)_2><01>}      {}
MMA_a01       =   C +  5H          + N  ; {@\FormatAq<MMA><01>}          {methylamine}
NH2CH2_a01    =   C +  4H          + N  ; {@\FormatAq<CH_2NH_2><01>}      {methylamine
radical}
HNCO_a01      =   C +   H +   0  + N  ; {@\FormatAq<HNCO><01>}          {ioscyanic
acid}
H2NCHO_a01    =   C +  3H +   0  + N  ; {@\FormatAq<H2NCHO><01>}          {formamide}
MMNNO2_a01    =   C +  2H +  20  + 2N  ; {@\FormatAq<MMNNO2><01>}      {methylnitramine}
MSIA_a01      =   C +  4H +   S + 20  ; {@\FormatAq<MSIA><01>}          {methyl
sulfinic acid}

{2C}
OXALAC_a01    =  IGNORE                ; {@\FormatAq<OXALAC><01>}          {oxalic acid,
2C + 2H + 40}
HCOCO2H_a01   =  2C +  2H  +  30      ; {@\FormatAq<HCOCO_2H><01>}          {oxoethanoic
acid}
HOCH2CHO_a01  =  2C +  4H  +  20      ; {@\FormatAq<HOCH_2CHO><01>}          {}
{glycolaldehyde}
HOCH2C(O)H_a01 =  2C +  4H  +  30      ; {@\FormatAq<HOCH_2CO_2H><01>}      {}
{hydroxyethanoic acid}
CH3C(O)O_a01  =  2C +  3H  +  30      ; {@\FormatAq<CH_3COO_2><01>}          {peroxyacetyl
radical}
GLYOX_a01     =  2C +  2H  +  20      ; {@\FormatAq<GLYOX><01>}          {CHOCHO =
glyoxal}
DMA_a01       =  2C +  7H          + N  ; {@\FormatAq<DMA><01>}          {}
{dimethylamine}
MEA_a01       =  2C +  7H  +   0  + N  ; {@\FormatAq<MEA><01>}          {ethanolamine}
MEANNO_a01    =  2C +  6H  +  20  + 2N  ; {@\FormatAq<MEANNO><01>}      {}
{ethanolamine}
MEANNO2_a01   =  2C +  6H  +  30  + 2N  ; {@\FormatAq<MEANNO2><01>}      {}
{ethanolamine}
NDMA_a01      =  2C +  6H  +   0  + 2N  ; {@\FormatAq<NDMA><01>}          {}
{N-nitroso
dimethylamine}
DMNNO2_a01    =  2C +  6H  +  20  + 2N  ; {@\FormatAq<DMNNO2><01>}      {}
{dimethylnitramine}
CH3NHCH2_a01  =  2C +  6H  +          N  ; {@\FormatAq<CH_3NHCH_2><01>}      {}
{methylamine
methyl radical}
CH3NHNHCH3_a01 =  2C +  8H  +          2N  ; {@\FormatAq<CH_3NHNHCH_3><01>}      {}
{dimethylhydrazine}
NH2C2H4NH2_a01 =  2C +  8H  +          2N  ; {@\FormatAq<NH_2CH_2CH_2NH_2><01>}      {}
{ethylenediamine}
NH2CH2CHOH_a01 =  2C +  6H  +   0  + N  ; {@\FormatAq<NH_2CH_2CHOH><01>}      {}
{ethanolamine
radical}
H2NCOCH2OH_a01 =  2C +  5H  +  20  + N  ; {@\FormatAq<H2NCOCH2OH><01>}      {}
{2-hydroxy
acetamide}
CH3NHCHO_a01  =  2C +  5H  +   0  + N  ; {@\FormatAq<CH_3NHCHO><01>}      {}
{N-methyl
formamide}
CH3NCO_a01    =  2C +  3H  +   0  + N  ; {@\FormatAq<CH_3NCO><01>}          {}
{methyl
isocyanic acid}
HPMTF_a01     =  2C +  4H  +  30  + S  ; {@\FormatAq<HPMTF><01>}          {}
{hydroperoxyl
methyl thioformate}

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H00CH2SCO_a01 = 2C + 3H + 30 + S ; {@\FormatAq<H00CH2SCO><01>} {}

{3C}
MGLYOX_a01 = 3C + 4H + 20 ; {@\FormatAq<MGLYOX><01>}
{methylglyoxal}
MGLYOAC_a01 = 3C + 4H + 30 ; {@\FormatAq<MGLYOAC><01>}
{methylglyoxylic acid}
DOC_a01 = IGNORE ; {@\FormatAq<DOC><01>} {dissolved
organic carbon DOC}
DOC0_a01 = IGNORE ; {@\FormatAq<DOC0><01>} {oxidized DOC}
TMA_a01 = 3C + 9H + N ; {@\FormatAq<TMA><01>}
{trimethylamine}
DMNCH2_a01 = 3C + 8H + N ; {@\FormatAq<(CH_3)_2NCH_2><01>}
{dimethylamine methyl radical}
DMNCHO_a01 = 3C + 7H + 0 + N ; {@\FormatAq<DMNCHO><01>} {N,N-dimethyl
formamide}
MALONAC_a01 = IGNORE ; {@\FormatAq<MALONAC><01>} {malonic
acid, 3C + 4H + 40}

{4C}
DEA_a01 = 4C + 11H + 20 + N ; {@\FormatAq<DEA><01>}
{diethanolamine}
NDELA_a01 = 4C + 10H + 30 + 2N ; {@\FormatAq<NDELA><01>} {N-nitroso
diethanolamine}
DEANNO2_a01 = 4C + 10H + 40 + 2N ; {@\FormatAq<DEANNO2><01>} {N-nitro
diethanolamine}
DEAN_a01 = 4C + 10H + 20 + N ; {@\FormatAq<HOETNHCH_2CHOH><01>}
{diethanolamine radical}
SUCCAC_a01 = IGNORE ; {@\FormatAq<SUCCAC><01>} {succinic
acid, 4C + 6H + 40}

{5C}
GLUTARAC_a01 = IGNORE ; {@\FormatAq<GLUTARAC><01>} {glutaric
acid, 5C + 8H + 40}

{6C}
TEA_a01 = 6C + 15H + 30 + N ; {@\FormatAq<TEA><01>}
{triethanolamine}
DENCH2CHOH_a01 = 6C + 14H + 30 + N ; {@\FormatAq<DENCH_2CHOH><01>}
{triethanolamine radical}
ADIPAC_a01 = IGNORE ; {@\FormatAq<ADIPAC><01>} {adipic acid,
6C + 10H + 40}

{----- ions -----}

{----- O -----}

{----- H -----}

{----- N -----}

{----- C -----}

{1C}
MMAp_a01 = C + 6H + N + Pls ; {@\FormatAq<MMA^+><01>}
{methylaminium}
MMNp_a01 = C + 5H + N + Pls ; {@\FormatAq<CH_3NH_2^+><01>}
{methylamine N-radical cation}
NH2CH2p_a01 = C + 4H + N + Pls ; {@\FormatAq<CH_2NH_2^+><01>}
{iminium}
NH3CH2p_a01 = C + 5H + N + Pls ; {@\FormatAq<CH_2NH_3^+><01>}
{methylaminium radical}
NCOm_a01 = C + 0 + N + Min ; {@\FormatAq<NCO^-><01>}
{isocyanate}

{2C}
HC204m_a01 = IGNORE + Min ; {@\FormatAq<HC_20_4^-><01>}

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{hydrogen oxalate, 2C + H + 40}
C2O4mm_a01 = IGNORE + 2Min ; {@\FormatAq<C_2O_4^<2->><01>}
{oxalate, 2C + 40}
HCOCO0m_a01 = 2C + H + 30 + Min ; {@\FormatAq<HCOCO0^-><01>} {}
MEAp_a01 = 2C + 8H + 0 + N + Pls ; {@\FormatAq<MEA^+><01>}
{ethanolaminium}
DMAp_a01 = 2C + 8H + N + Pls ; {@\FormatAq<DMA^+><01>}
{dimethylaminium}
DMNp_a01 = 2C + 7H + N + Pls ; {@\FormatAq<(CH_3)_2NH^+><01>}
{dimethylamine N-radical cation}
CH3NHCH2p_a01 = 2C + 6H + N + Pls ; {@\FormatAq<CH_3NH^+CH_2><01>}
{methyl iminium}
CH3NH2CH2p_a01 = 2C + 7H + N + Pls ; {@\FormatAq<CH_3NH_2^+CH_2><01>}
{dimethylaminium radical}
MENp_a01 = 2C + 7H + 0 + N + Pls ; {@\FormatAq<HOCH_2CH_2NH_2^+><01>}
{ethanolamine N-radical cation}
NH3CH2CHOHp_a01 = 2C + 7H + 0 + N + Pls ; {@\FormatAq<HOCHCH_2NH_3^+><01>}
{ethanolaminium radical}

{3C}
CH3COC00m_a01 = 3C + 3H + 30 + Min ; {@\FormatAq<CH_3COC00^-><01>}
{methylglyoxalate}
TMAp_a01 = 3C + 10H + N + Pls ; {@\FormatAq<TMA^+><01>}
{trimethylaminium}
TMNp_a01 = 3C + 9H + N + Pls ; {@\FormatAq<(CH_3)_3N^+><01>}
{trimethylamine N-radical cation}
DMNCH2p_a01 = 3C + 8H + N + Pls ; {@\FormatAq<(CH_3)_2NH^+CH_2><01>}
{dimethyl iminium}
DMNHCH2p_a01 = 3C + 9H + N + Pls ; {@\FormatAq<(CH_3)_2NH^+CH_2><01>}
{trimethylaminium radical}

{4C}
DEAp_a01 = 4C + 12H + 20 + N + Pls ; {@\FormatAq<DEA^+><01>}
{diethanolaminium}
DENp_a01 = 4C + 13H + 20 + N + Pls ; {@\FormatAq<(HOET)_2NH^+><01>}
{diethanolamine N-radical cation}
DENHp_a01 = 4C + 12H + 20 + N + Pls ; {@\FormatAq<HOETNH_2CH_2CHOH^+><01>}
{diethanolaminium radical}
C2H5C2O4m_a01 = IGNORE + Min ; {@\FormatAq<CH_2CH_2HC_2O_4^-><01>}
{hydrogen succinate, 4C + 5H + 40}
C2H4C2O4mm_a01 = IGNORE + 2Min ; {@\FormatAq<CH_2CH_2C_2O_4^<2->><01>}
{succinate, 4C + 4H + 40}

{6C}
TEAp_a01 = 6C + 16H + 30 + N + Pls ; {@\FormatAq<TEA^+><01>}
{triethanolaminium}
TENp_a01 = 6C + 15H + 30 + N + Pls ; {@\FormatAq<(HOET)_3N^+><01>}
{triethanolamine N-radical cation}
DENIMp_a01 = 6C + 15H + 30 + N + Pls ; {@\FormatAq<(HOET)_2N^+CH_2CH_2OH><01>}
{diethanol iminium}
TENHp_a01 = 6C + 15H + 30 + N + Pls ; {@\FormatAq<(HOET)_2NH^+CH_2CHOH><01>}
{triethanolaminium radical}

{-----M-----}
{**** END: aerosol species (phase 1) from aqueous.spc ****}
{**** START: aerosol species (phase 2) from aqueous.spc ****}
{-----}
{----- aerosol mode: 02 -----}
{-----}

{----- neutral species -----}

{----- 0 -----}

02_a02 = 20 ; {@\FormatAq<O_2><02>} {oxygen}
03_a02 = 30 ; {@\FormatAq<O_3><02>} {ozone}

{----- H -----}

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OH_a02	= H + 0	; {@\FormatAq<OH><02>}	{hydroxyl radical}
H02_a02	= H + 20	; {@\FormatAq<H0_2><02>}	{perhydroxyl}
radical}			
H20_a02	= 2H + 0	; {@\FormatAq<H_20><02>}	{water}
H202_a02	= 2H + 20	; {@\FormatAq<H_20_2><02>}	{hydrogen peroxide}

{----- N -----}

NH3_a02	= 3H + N	; {@\FormatAq<NH_3><02>}	{ammonia}
N0_a02	= 0 + N	; {@\FormatAq<N0><02>}	{nitric oxide}
N02_a02	= 20 + N	; {@\FormatAq<N0_2><02>}	{nitrogen dioxide}
N03_a02	= 30 + N	; {@\FormatAq<N0_3><02>}	{nitrogen trioxide}
HON0_a02	= H + 20 + N	; {@\FormatAq<HON0><02>}	{nitrous acid}
HN03_a02	= H + 30 + N	; {@\FormatAq<HNO_3><02>}	{nitric acid}
HN04_a02	= H + 40 + N	; {@\FormatAq<HNO_4><02>}	{pernitric acid}

{----- C -----}

{1C}			
CH3OH_a02	= C + 4H + 0	; {@\FormatAq<CH_3OH><02>}	{methanol}
HC00H_a02	= C + 2H + 20	; {@\FormatAq<HC00H><02>}	{formic acid}
HCH0_a02	= C + 2H + 0	; {@\FormatAq<HCH0><02>}	{methanal}
(formaldehyde)}			
CH302_a02	= C + 3H + 20	; {@\FormatAq<CH_300><02>}	{methylperoxy}
radical}			
CH300H_a02	= C + 4H + 20	; {@\FormatAq<CH_300H><02>}	{}
C02_a02	= C + 20	; {@\FormatAq<C0_2><02>}	{carbon dioxide}

{2C}			
CH3C02H_a02	= 2C + 4H + 20	; {@\FormatAq<CH_3C00H><02>}	{acetic acid}
PAN_a02	= 2C + 3H + 50 + N	; {@\FormatAq<PAN><02>}	
{peroxyacetylnitrate}			
CH3CH0_a02	= 2C + 4H + 0	; {@\FormatAq<CH_3CH0><02>}	{acetaldehyde}

{3C}			
CH3C0CH3_a02	= 3C + 6H + 0	; {@\FormatAq<CH_3C0CH_3><02>}	{acetone}

{----- Cl -----}

Cl_a02	= Cl	; {@\FormatAq<Cl><02>}	{chlorine atom}
Cl2_a02	= 2Cl	; {@\FormatAq<Cl_2><02>}	{molecular}
chlorine}			
HCl_a02	= H + Cl	; {@\FormatAq<HCl><02>}	{hydrogen chloride}
HOCl_a02	= H + 0 + Cl	; {@\FormatAq<HOCl><02>}	{hypochlorous acid}

{----- Br -----}

Br_a02	= Br	; {@\FormatAq <02>}	{bromine atom}
Br2_a02	= 2Br	; {@\FormatAq<Br_2><02>}	{molecular bromine}
HBr_a02	= H + Br	; {@\FormatAq<HBr><02>}	{hydrogen bromide}
HOBr_a02	= H + 0 + Br	; {@\FormatAq<HOBr><02>}	{hypobromous acid}
BrCl_a02	= Br + Cl	; {@\FormatAq<BrCl><02>}	{bromine chloride}

{----- I -----}

I2_a02	= 2I	; {@\FormatAq<I_2><02>}	{molecular iodine}
I0_a02	= I + 0	; {@\FormatAq<I0><02>}	{iodine monoxide}
radical}			
HOI_a02	= H + 0 + I	; {@\FormatAq<HOI><02>}	{hypoiodous acid}
ICl_a02	= I + Cl	; {@\FormatAq<ICl><02>}	{iodine chloride}
IBr_a02	= I + Br	; {@\FormatAq<IBr><02>}	{iodine bromide}

{----- S -----}

S02_a02	= S + 20	; {@\FormatAq<S0_2><02>}	{sulfur dioxide}
H2S04_a02	= 2H + S + 40	; {@\FormatAq<H_2S0_4><02>}	{sulfuric acid}
DMS_a02	= 2C + 6H + S	; {@\FormatAq<DMS><02>}	{dimethyl sulfide}
CH3SCH3}			

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DMSO_a02      = 2C + 6H + S + O      ; {@\FormatAq<DMSO><02>}      {dimethyl
sulfoxide: CH3SOCH3}

{----- Hg -----}

Hg_a02        = Hg                    ; {@\FormatAq<Hg><02>}      {mercury}
Hg0_a02       = Hg + 0                ; {@\FormatAq<Hg0><02>}      {}
HgOH0H_a02    = Hg + 2O + 2H          ; {@\FormatAq<Hg(OH)_2><02>} {}
HgOHC1_a02    = Hg + 0 + H + Cl       ; {@\FormatAq<Hg(OH)Cl><02>} {}
HgCl2_a02     = Hg + 2Cl              ; {@\FormatAq<HgCl_2><02>} {}
HgBr2_a02     = Hg + 2Br              ; {@\FormatAq<HgBr_2><02>} {}
HgSO3_a02     = Hg + S + 3O           ; {@\FormatAq<HgSO_3><02>} {}
ClHgBr_a02    = Hg + Cl + Br          ; {@\FormatAq<ClHgBr><02>} {}
BrHgOBr_a02   = Hg + 0 + 2Br         ; {@\FormatAq<BrHgOBr><02>} {}
ClHgOBr_a02   = Hg + 0 + Cl + Br     ; {@\FormatAq<ClHgOBr><02>} {}

{----- Fe -----}

FeOH3_a02     = Fe + 3O + 3H          ; {@\FormatAq<FeOH3><02>} {}
FeCl3_a02     = Fe + 3Cl              ; {@\FormatAq<FeCl3><02>} {}
FeF3_a02      = Fe + 3F               ; {@\FormatAq<FeF3><02>} {}

{----- ions -----}

{----- O -----}

O2m_a02       = 2O                    + Min ; {@\FormatAq<O_2^-><02>} {}
OHm_a02       = H + 0                  + Min ; {@\FormatAq<OH^-><02>} {}
HO2m_a02      = H + 2O                  + Min ; {@\FormatAq<HO2^-><02>} {}
O2mm_a02      = 2O                      + 2Min ; {@\FormatAq<O2^<2->><02>} {}

{----- H -----}

Hp_a02        = H                      + Pls ; {@\FormatAq<H^+><02>} {}

{----- N -----}

NH4p_a02      = N + 4H                  + Pls ; {@\FormatAq<NH_4^+><02>} {ammonium}
NO2m_a02      = 2O + N                  + Min ; {@\FormatAq<NO_2^-><02>} {nitrite}
NO3m_a02      = 3O + N                  + Min ; {@\FormatAq<NO_3^-><02>} {nitrate}
NO4m_a02      = 4O + N                  + Min ; {@\FormatAq<NO_4^-><02>} {peroxy nitrate}

{----- C -----}

{1C}
CO3m_a02      = C + 3O                  + Min ; {@\FormatAq<CO_3^-><02>} {}
HCO0m_a02     = H + C + 2O              + Min ; {@\FormatAq<HCO0^-><02>} {formate}
HCO3m_a02     = H + C + 3O              + Min ; {@\FormatAq<HCO_3^-><02>} {hydrogen
carbonate}

{2C}
CH3CO0m_a02   = 2C + 3H + 2O            + Min ; {@\FormatAq<CH_3CO0^-><02>} {acetate}

{----- Cl -----}

Clm_a02       = Cl                      + Min ; {@\FormatAq<Cl^-><02>} {chloride}
Cl2m_a02      = 2Cl                     + Min ; {@\FormatAq<Cl_2^-><02>} {}
Cl0m_a02      = Cl + 0                  + Min ; {@\FormatAq<Cl0^-><02>} {}
ClOHm_a02     = H + 0 + Cl              + Min ; {@\FormatAq<ClOH^-><02>} {}

{----- Br -----}

Brm_a02       = Br                      + Min ; {@\FormatAq<Br^-><02>} {bromide}
Br2m_a02      = 2Br                     + Min ; {@\FormatAq<Br_2^-><02>} {}
Br0m_a02      = Br + 0                  + Min ; {@\FormatAq<Br0^-><02>} {}
BrOHm_a02     = H + 0 + Br              + Min ; {@\FormatAq<BrOH^-><02>} {}
BrCl2m_a02    = Br + 2Cl                + Min ; {@\FormatAq<BrCl_2^-><02>} {}
Br2Clm_a02    = 2Br + Cl                + Min ; {@\FormatAq<Br_2Cl^-><02>} {}

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{----- I -----}

Im_a02      = I          + Min ; {@\FormatAq<I^-><02>}      {iodide}
IO2m_a02    = I + 20      + Min ; {@\FormatAq<IO_2^-><02>}    {}
IO3m_a02    = I + 30      + Min ; {@\FormatAq<IO_3^-><02>}    {iodate}
ICl2m_a02   = I + 2Cl     + Min ; {@\FormatAq<ICl_2^-><02>}   {}
IBr2m_a02   = I + 2Br     + Min ; {@\FormatAq<IBr_2^-><02>}   {}

{----- S -----}

SO3m_a02     = S + 30      + Min ; {@\FormatAq<SO_3^-><02>}      {}
SO3mm_a02    = S + 30      + 2Min ; {@\FormatAq<SO_3^-><2><02>} {sulfite}
SO4m_a02     = S + 40      + Min ; {@\FormatAq<SO_4^-><02>}      {}
SO4mm_a02    = S + 40      + 2Min ; {@\FormatAq<SO_4^-><2><02>} {sulfate}
SO5m_a02     = S + 50      + Min ; {@\FormatAq<SO_5^-><02>}      {}
HSO3m_a02    = H + S + 30  + Min ; {@\FormatAq<HSO_3^-><02>}   {hydrogen sulfite}
HSO4m_a02    = H + S + 40  + Min ; {@\FormatAq<HSO_4^-><02>}   {hydrogen sulfate}
HSO5m_a02    = H + S + 50  + Min ; {@\FormatAq<HSO_5^-><02>}   {}
CH3SO3m_a02  = C + 3H + S + 30 + Min ; {@\FormatAq<CH_3SO_3^-><02>} {MSA anion}
CH2OHSO3m_a02 = C + 3H + S + 40 + Min ; {@\FormatAq<CH_2OHSO_3^-><02>} {}

{----- Hg -----}

Hgp_a02      = Hg          + Pls ; {@\FormatAq<Hg^+><02>}      {}
Hgpp_a02     = Hg          + 2Pls ; {@\FormatAq<Hg^+><2><02>}   {}
HgOHp_a02    = Hg + 0 + H  + Pls ; {@\FormatAq<HgOH^+><02>}    {}
HgClp_a02    = Hg + Cl     + Pls ; {@\FormatAq<HgCl^+><02>}    {}
HgBrp_a02    = Hg + Br     + Pls ; {@\FormatAq<HgBr^+><02>}    {}
HgSO32mm_a02 = Hg + 2S + 60 + 2Min ; {@\FormatAq<Hg(SO_3)_2^-><2><02>} {}

{----- Fe -----}

Fepp_a02     = Fe          + 2Pls ; {@\FormatAq<Fe^+><2><02>}   {Fe(II)}
FeOpp_a02    = Fe + 0      + 2Pls ; {@\FormatAq<Fe0^+><2><02>}   {Fe(II)}
FeOHp_a02    = Fe + 0 + H  + Pls ; {@\FormatAq<FeOH^+><02>}     {Fe(II)}
FeOH2p_a02   = Fe + 20 + 2H + Pls ; {@\FormatAq<Fe(OH)_2^+><02>} {Fe(II)}
FeClp_a02    = Fe + Cl     + Pls ; {@\FormatAq<FeCl^+><02>}     {Fe(II)}
Feppp_a02    = Fe          + 3Pls ; {@\FormatAq<Fe^+><3><02>}   {Fe(III)}
FeH0pp_a02   = Fe + 0 + H  + 2Pls ; {@\FormatAq<FeH0^+><2><02>} {Fe(III)}
FeH02pp_a02  = Fe + 20 + H  + 2Pls ; {@\FormatAq<FeH0_2^+><2><02>} {Fe(III)}
FeOHpp_a02   = Fe + 0 + H  + 2Pls ; {@\FormatAq<FeOH^+><2><02>} {Fe(III)}
FeOH4m_a02   = Fe + 40 + 4H + Min ; {@\FormatAq<Fe(OH)_4^-><02>} {Fe(III)}
FeOHH02p_a02 = Fe + 30 + 2H + Pls ; {@\FormatAq<Fe(OH)(H0_2)^+><02>} {Fe(III)}
FeClpp_a02   = Fe + Cl     + 2Pls ; {@\FormatAq<FeCl^+><2><02>} {Fe(III)}
FeCl2p_a02   = Fe + 2Cl    + Pls ; {@\FormatAq<FeCl_2^+><02>} {Fe(III)}
FeBrpp_a02   = Fe + Br     + 2Pls ; {@\FormatAq<FeBr^+><2><02>} {Fe(III)}
FeBr2p_a02   = Fe + 2Br    + Pls ; {@\FormatAq<FeBr_2^+><02>} {Fe(III)}
FeFpp_a02    = Fe + F      + 2Pls ; {@\FormatAq<FeF^+><2><02>} {Fe(III)}
FeF2p_a02    = Fe + 2F     + 2Pls ; {@\FormatAq<FeF_2^+><02>} {Fe(III)}
FeS03p_a02   = Fe + 30 + S  + Pls ; {@\FormatAq<FeSO_3^+><02>} {Fe(III)}
FeS04p_a02   = Fe + 40 + S  + Pls ; {@\FormatAq<FeSO_4^+><02>} {Fe(III)}
FeS042m_a02  = Fe + 80 + 2S + Min ; {@\FormatAq<Fe(SO_4)_2^-><02>} {Fe(III)}
FeOH2Fepppp_a02 = 2 Fe + 0 + H + 4Pls ; {@\FormatAq<Fe(OH)_2Fe^+><4><02>} {Fe(III)}

{----- dummies -----}

D10_a02      = Ignore      ; {@\FormatAq<D_10><02>}      {}
Nap_a02      = Ignore      ; {@\FormatAq<Na^+><02>}      {dummy cation}

{----- aerosol mode: 02 -----}

{----- neutral species -----}

{----- 0 -----}

{----- H -----}

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{----- N -----}
N2O3_a02      =          30 + 2N ; {@\FormatAq<N_2O3><02>}      {dinitrogen
trioxide}
N2O4_a02      =          40 + 2N ; {@\FormatAq<N_2O4><02>}      {dinitrogen
tetraoxide}

{----- C -----}

{1C}
CH2O2H2_a02   =   C + 4H + 20      ; {@\FormatAq<CH2(OH)2><02>}      {}
MMA_a02       =   C + 5H          + N ; {@\FormatAq<MMA><02>}      {methylamine}
NH2CH2_a02    =   C + 4H          + N ; {@\FormatAq<CH2NH2><02>}      {methylamine
radical}
HNCO_a02      =   C +  H +  0 + N ; {@\FormatAq<HNCO><02>}      {ioscyanic
acid}
H2NCHO_a02    =   C + 3H +  0 + N ; {@\FormatAq<H2NCHO><02>}      {formamide}
MMNNO2_a02    =   C + 2H + 20 + 2N ; {@\FormatAq<MMNNO2><02>}      {methylnitramine}
MSIA_a02      =   C + 4H +  S + 20 ; {@\FormatAq<MSIA><02>}      {methyl
sulfinic acid}

{2C}
OXALAC_a02    =  IGNORE                ; {@\FormatAq<OXALAC><02>}      {oxalic acid,
2C + 2H + 40}
HCOCO2H_a02   =  2C + 2H + 30          ; {@\FormatAq<HCOCO2H><02>}      {oxoethanoic
acid}
HOCH2CHO_a02  =  2C + 4H + 20          ; {@\FormatAq<HOCH2CHO><02>}      {}
{glycolaldehyde}
HOCH2CO2H_a02 =  2C + 4H + 30          ; {@\FormatAq<HOCH2CO2H><02>}      {}
{hydroxyethanoic acid}
CH3CO3_a02    =  2C + 3H + 30          ; {@\FormatAq<CH3CO3><02>}      {peroxyacetyl
radical}
GLYOX_a02     =  2C + 2H + 20          ; {@\FormatAq<GLYOX><02>}      {CHOCHO =
glyoxal}
DMA_a02       =  2C + 7H          + N ; {@\FormatAq<DMA><02>}      {}
{dimethylamine}
MEA_a02       =  2C + 7H +  0 + N ; {@\FormatAq<MEA><02>}      {ethanolamine}
MEANNO_a02    =  2C + 6H + 20 + 2N ; {@\FormatAq<MEANNO><02>}      {N-nitroso
ethanolamine}
MEANNO2_a02   =  2C + 6H + 30 + 2N ; {@\FormatAq<MEANNO2><02>}      {N-nitro
ethanolamine}
NDMA_a02      =  2C + 6H +  0 + 2N ; {@\FormatAq<NDMA><02>}      {N-nitroso
dimethylamine}
DMNNO2_a02    =  2C + 6H + 20 + 2N ; {@\FormatAq<DMNNO2><02>}      {}
{dimethylnitramine}
CH3NHCH2_a02  =  2C + 6H +          N ; {@\FormatAq<CH3NHCH2><02>}      {methylamine
methyl radical}
CH3NHNHCH3_a02 =  2C + 8H +          2N ; {@\FormatAq<CH3NHNHCH3><02>}      {}
{dimethylhydrazine}
NH2C2H4NH2_a02 =  2C + 8H +          2N ; {@\FormatAq<NH2CH2CH2NH2><02>}      {}
{ethylenediamine}
NH2CH2CHOH_a02 =  2C + 6H +  0 + N ; {@\FormatAq<NH2CH2CHOH><02>}      {ethanolamine
radical}
H2NCOCH2OH_a02 =  2C + 5H + 20 + N ; {@\FormatAq<H2NCOCH2OH><02>}      {2-hydroxy
acetamide}
CH3NHCHO_a02  =  2C + 5H +  0 + N ; {@\FormatAq<CH3NHCHO><02>}      {N-methyl
formamide}
CH3NCO_a02    =  2C + 3H +  0 + N ; {@\FormatAq<CH3NCO><02>}      {methyl
isocyanic acid}
HPMTF_a02     =  2C + 4H + 30 + S ; {@\FormatAq<HPMTF><02>}      {hydroperoxyl
methyl thioformate}
HOOCH2SCO_a02 =  2C + 3H + 30 + S ; {@\FormatAq<HOOCH2SCO><02>}      {}

{3C}
MGLYOX_a02    =  3C + 4H + 20          ; {@\FormatAq<MGLYOX><02>}      {}
{methylglyoxal}
MGLYOAC_a02   =  3C + 4H + 30          ; {@\FormatAq<MGLYOAC><02>}      {}
{methylglyoxylic acid}

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DOC_a02 = IGNORE ; {@\FormatAq<DOC><02>} {dissolved
 organic carbon DOC}
 DOCO_a02 = IGNORE ; {@\FormatAq<DOCO><02>} {oxidized DOC}
 TMA_a02 = 3C + 9H + N ; {@\FormatAq<TMA><02>}
 {trimethylamine}
 DMNCH2_a02 = 3C + 8H + N ; {@\FormatAq<(CH_3)_2NCH_2><02>}
 {dimethylamine methyl radical}
 DMNCHO_a02 = 3C + 7H + 0 + N ; {@\FormatAq<DMNCHO><02>} {N,N-dimethyl
 formamide}
 MALONAC_a02 = IGNORE ; {@\FormatAq<MALONAC><02>} {malonic
 acid, 3C + 4H + 4O}

 {4C}
 DEA_a02 = 4C + 11H + 20 + N ; {@\FormatAq<DEA><02>}
 {diethanolamine}
 NDELA_a02 = 4C + 10H + 30 + 2N ; {@\FormatAq<NDELA><02>} {N-nitroso
 diethanolamine}
 DEANN02_a02 = 4C + 10H + 40 + 2N ; {@\FormatAq<DEANN02><02>} {N-nitro
 diethanolamine}
 DEAN_a02 = 4C + 10H + 20 + N ; {@\FormatAq<HOETNHCH_2CHOH><02>}
 {diethanolamine radical}
 SUCCAC_a02 = IGNORE ; {@\FormatAq<SUCCAC><02>} {succinic
 acid, 4C + 6H + 4O}

 {5C}
 GLUTARAC_a02 = IGNORE ; {@\FormatAq<GLUTARAC><02>} {glutaric
 acid, 5C + 8H + 4O}

 {6C}
 TEA_a02 = 6C + 15H + 30 + N ; {@\FormatAq<TEA><02>}
 {triethanolamine}
 DENCH2CHOH_a02 = 6C + 14H + 30 + N ; {@\FormatAq<DENCH_2CHOH><02>}
 {triethanolamine radical}
 ADIPAC_a02 = IGNORE ; {@\FormatAq<ADIPAC><02>} {adipic acid,
 6C + 10H + 4O}

 {----- ions -----}
 {----- O -----}
 {----- H -----}
 {----- N -----}
 {----- C -----}

 {1C}
 MMAp_a02 = C + 6H + N + Pls ; {@\FormatAq<MMA^+><02>}
 {methylaminium}
 MMNp_a02 = C + 5H + N + Pls ; {@\FormatAq<CH_3NH_2^+><02>}
 {methylamine N-radical cation}
 NH2CH2p_a02 = C + 4H + N + Pls ; {@\FormatAq<CH_2NH_2^+><02>}
 {iminium}
 NH3CH2p_a02 = C + 5H + N + Pls ; {@\FormatAq<CH_2NH_3^+><02>}
 {methylaminium radical}
 NCOm_a02 = C + 0 + N + Min ; {@\FormatAq<NCO^-><02>}
 {isocyanate}

 {2C}
 HC204m_a02 = IGNORE + Min ; {@\FormatAq<HC_20_4^-><02>}
 {hydrogen oxalate, 2C + H + 4O}
 C204mm_a02 = IGNORE + 2Min ; {@\FormatAq<C_20_4^<2->><02>}
 {oxalate, 2C + 4O}
 HCOCO0m_a02 = 2C + H + 30 + Min ; {@\FormatAq<HCOCO0^><02>} {}
 MEAp_a02 = 2C + 8H + 0 + N + Pls ; {@\FormatAq<MEA^+><02>}
 {ethanolaminium}
 DMAp_a02 = 2C + 8H + N + Pls ; {@\FormatAq<DMA^+><02>}


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{dimethylaminium}
DMNp_a02      = 2C + 7H          + N + Pls ; {@\FormatAq<(CH_3)_2NH^+><02>}
{dimethylamine N-radical cation}
CH3NHCH2p_a02 = 2C + 6H          + N + Pls ; {@\FormatAq<CH_3NH^+CH_2><02>}
{methyl iminium}
CH3NH2CH2p_a02 = 2C + 7H          + N + Pls ; {@\FormatAq<CH_3NH_2^+CH_2><02>}
{dimethylaminium radical}
MENp_a02      = 2C + 7H + 0      + N + Pls ; {@\FormatAq<HOCH_2CH_2NH_2^+><02>}
{ethanolamine N-radical cation}
NH3CH2CHOHp_a02 = 2C + 7H + 0      + N + Pls ; {@\FormatAq<HOCHCH_2NH_3^+><02>}
{ethanolaminium radical}

{3C}
CH3COCOOm_a02 = 3C + 3H + 30      + Min ; {@\FormatAq<CH_3COCOO^-><02>}
{methylglyoxalate}
TMAp_a02      = 3C + 10H         + N + Pls ; {@\FormatAq<TMA^+><02>}
{trimethylaminium}
TMNp_a02      = 3C + 9H          + N + Pls ; {@\FormatAq<(CH_3)_3N^+><02>}
{trimethylamine N-radical cation}
DMNCH2p_a02   = 3C + 8H          + N + Pls ; {@\FormatAq<(CH_3)_2N^+CH_2><02>}
{dimethyl iminium}
DMNHCH2p_a02  = 3C + 9H          + N + Pls ; {@\FormatAq<(CH_3)_2NH^+CH_2><02>}
{trimethylaminium radical}

{4C}
DEAp_a02      = 4C + 12H + 20      + N + Pls ; {@\FormatAq<DEA^+><02>}
{diethanolaminium}
DENp_a02      = 4C + 13H + 20      + N + Pls ; {@\FormatAq<(HOET)_2NH^+><02>}
{diethanolamine N-radical cation}
DENHp_a02     = 4C + 12H + 20      + N + Pls ; {@\FormatAq<HOETNH_2CH_2CHOH^+><02>}
{diethanolaminium radical}
C2H5C2O4m_a02 = IGNORE          + Min ; {@\FormatAq<CH_2CH_2HC_2O_4^-><02>}
{hydrogen succinate, 4C + 5H + 40}
C2H4C2O4mm_a02 = IGNORE          + 2Min ; {@\FormatAq<CH_2CH_2C_2O_4^<2->><02>}
{succinate, 4C + 4H + 40}

{6C}
TEAp_a02      = 6C + 16H + 30      + N + Pls ; {@\FormatAq<TEA^+><02>}
{triethanolaminium}
TENp_a02      = 6C + 15H + 30      + N + Pls ; {@\FormatAq<(HOET)_3N^+><02>}
{triethanolamine N-radical cation}
DENIMp_a02    = 6C + 15H + 30      + N + Pls ; {@\FormatAq<(HOET)_2N^+CH_2CH_2OH><02>}
{diethanol iminium}
TENHp_a02     = 6C + 15H + 30      + N + Pls ; {@\FormatAq<(HOET)_2NH^+CH_2CHOH><02>}
{triethanolaminium radical}

{-----M-----}
{**** END: aerosol species (phase 2) from aqueous.spc ****}
{**** START: aerosol species (phase 3) from aqueous.spc ****}
{-----}
{----- aerosol mode: 03 -----}
{-----}

{----- neutral species -----}

{----- 0 -----}

O2_a03        = 20                ; {@\FormatAq<O_2><03>}          {oxygen}
O3_a03        = 30                ; {@\FormatAq<O_3><03>}          {ozone}

{-----H-----}

OH_a03        = H + 0              ; {@\FormatAq<OH><03>}          {hydroxyl radical}
HO2_a03       = H + 20             ; {@\FormatAq<HO_2><03>}       {perhydroxyl radical}
H2O_a03       = 2H + 0             ; {@\FormatAq<H_2O><03>}       {water}
H2O2_a03      = 2H + 20            ; {@\FormatAq<H_2O_2><03>}     {hydrogen peroxide}

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{----- N -----}

NH3_a03      = 3H      + N      ; {@\FormatAq<NH_3><03>}      {ammonia}
NO_a03       =      0 + N      ; {@\FormatAq<NO><03>}       {nitric oxide}
NO2_a03      =      20 + N      ; {@\FormatAq<NO_2><03>}      {nitrogen dioxide}
NO3_a03      =      30 + N      ; {@\FormatAq<NO_3><03>}      {nitrogen trioxide}
HONO_a03     = H + 20 + N      ; {@\FormatAq<HONO><03>}     {nitrous acid}
HNO3_a03     = H + 30 + N      ; {@\FormatAq<HNO_3><03>}    {nitric acid}
HNO4_a03     = H + 40 + N      ; {@\FormatAq<HNO_4><03>}    {pernitric acid}

{----- C -----}

{1C}
CH3OH_a03    = C + 4H + 0      ; {@\FormatAq<CH_3OH><03>}    {methanol}
HCOOH_a03    = C + 2H + 20     ; {@\FormatAq<HCOOH><03>}    {formic acid}
HCHO_a03     = C + 2H + 0      ; {@\FormatAq<HCHO><03>}     {methanal}
(formaldehyde)}
CH3O2_a03    = C + 3H + 20     ; {@\FormatAq<CH_3O2><03>}    {methylperoxy
radical}
CH3OOH_a03   = C + 4H + 20     ; {@\FormatAq<CH_3OOH><03>}   {}
CO2_a03      = C      + 20     ; {@\FormatAq<CO_2><03>}     {carbon dioxide}

{2C}
CH3CO2H_a03  = 2C + 4H + 20     ; {@\FormatAq<CH_3COOH><03>}  {acetic acid}
PAN_a03      = 2C + 3H + 50 + N ; {@\FormatAq<PAN><03>}      {}
{peroxyacetylnitrate}
CH3CHO_a03   = 2C + 4H + 0      ; {@\FormatAq<CH_3CHO><03>}   {acetaldehyde}

{3C}
CH3COCH3_a03 = 3C + 6H + 0      ; {@\FormatAq<CH_3COCH_3><03>} {acetone}

{----- Cl -----}

Cl_a03       = Cl              ; {@\FormatAq<Cl><03>}        {chlorine atom}
Cl2_a03      = 2Cl             ; {@\FormatAq<Cl_2><03>}      {molecular
chlorine}
HCl_a03      = H + Cl          ; {@\FormatAq<HCl><03>}       {hydrogen chloride}
HOCl_a03     = H + 0 + Cl      ; {@\FormatAq<HOCl><03>}      {hypochlorous acid}

{----- Br -----}

Br_a03       = Br              ; {@\FormatAq<Br><03>}        {bromine atom}
Br2_a03      = 2Br             ; {@\FormatAq<Br_2><03>}      {molecular bromine}
HBr_a03      = H + Br          ; {@\FormatAq<HBr><03>}       {hydrogen bromide}
HOBr_a03     = H + 0 + Br      ; {@\FormatAq<HOBr><03>}      {hypobromous acid}
BrCl_a03     = Br + Cl         ; {@\FormatAq<BrCl><03>}      {bromine chloride}

{----- I -----}

I2_a03       = 2I              ; {@\FormatAq<I_2><03>}       {molecular iodine}
IO_a03       = I + 0           ; {@\FormatAq<IO><03>}        {iodine monoxide
radical}
HOI_a03      = H + 0 + I       ; {@\FormatAq<HOI><03>}       {hypoiodous acid}
ICl_a03      = I + Cl          ; {@\FormatAq<ICl><03>}       {iodine chloride}
IBr_a03      = I + Br          ; {@\FormatAq<IBr><03>}       {iodine bromide}

{----- S -----}

SO2_a03      = S + 20          ; {@\FormatAq<SO_2><03>}      {sulfur dioxide}
H2SO4_a03    = 2H + S + 40     ; {@\FormatAq<H_2SO_4><03>}   {sulfuric acid}
DMS_a03      = 2C + 6H + S     ; {@\FormatAq<DMS><03>}       {dimethyl sulfide:
CH3SCH3}
DMSO_a03     = 2C + 6H + S + 0 ; {@\FormatAq<DMSO><03>}      {dimethyl
sulfoxide: CH3SOCH3}

{----- Hg -----}

Hg_a03       = Hg              ; {@\FormatAq<Hg><03>}        {mercury}
Hg0_a03      = Hg + 0          ; {@\FormatAq<Hg0><03>}       {}

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HgOH ₂	= Hg + 2O + 2H	; { @\FormatAq<Hg(OH) ₂ ><03> }	{ }
HgOHCl	= Hg + O + H + Cl	; { @\FormatAq<Hg(OH)Cl><03> }	{ }
HgCl ₂	= Hg + 2Cl	; { @\FormatAq<HgCl ₂ ><03> }	{ }
HgBr ₂	= Hg + 2Br	; { @\FormatAq<HgBr ₂ ><03> }	{ }
HgSO ₃	= Hg + S + 3O	; { @\FormatAq<HgSO ₃ ><03> }	{ }
ClHgBr	= Hg + Cl + Br	; { @\FormatAq<ClHgBr><03> }	{ }
BrHgOBr	= Hg + O + 2Br	; { @\FormatAq<BrHgOBr><03> }	{ }
ClHgOBr	= Hg + O + Cl + Br	; { @\FormatAq<ClHgOBr><03> }	{ }

{-----Fe-----}

FeOH ₃	= Fe + 3O + 3H	; { @\FormatAq<FeOH ₃ ><03> }	{ }
FeCl ₃	= Fe + 3Cl	; { @\FormatAq<FeCl ₃ ><03> }	{ }
FeF ₃	= Fe + 3F	; { @\FormatAq<FeF ₃ ><03> }	{ }

{----- ions -----}

{----- O -----}

O _{2m}	= 2O	+ Min ; { @\FormatAq<O ₂ ><03> }	{ }
OH _m	= H + O	+ Min ; { @\FormatAq<OH><03> }	{ }
H ₂ O _{2m}	= H + 2O	+ Min ; { @\FormatAq<H ₂ O ₂ ><03> }	{ }
O _{2mm}	= 2O	+ 2Min ; { @\FormatAq<O ₂ ²⁻ ><03> }	{ }

{----- H -----}

H _p	= H	+ Pls ; { @\FormatAq<H><03> }	{ }
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{----- N -----}

NH _{4p}	= N + 4H	+ Pls ; { @\FormatAq<NH ₄ ><03> }	{ ammonium }
NO _{2m}	= 2O + N	+ Min ; { @\FormatAq<NO ₂ ><03> }	{ nitrite }
NO _{3m}	= 3O + N	+ Min ; { @\FormatAq<NO ₃ ><03> }	{ nitrate }
NO _{4m}	= 4O + N	+ Min ; { @\FormatAq<NO ₄ ><03> }	{ peroxy nitrate }

{----- C -----}

{1C}			
CO _{3m}	= C + 3O	+ Min ; { @\FormatAq<CO ₃ ><03> }	{ }
HCO _{0m}	= H + C + 2O	+ Min ; { @\FormatAq<HCO ₀ ><03> }	{ formate }
HCO _{3m}	= H + C + 3O	+ Min ; { @\FormatAq<HCO ₃ ><03> }	{ hydrogen carbonate }

{2C}			
CH ₃ CO _{0m}	= 2C + 3H + 2O	+ Min ; { @\FormatAq<CH ₃ CO ₀ ><03> }	{ acetate }

{----- Cl -----}

Cl _m	= Cl	+ Min ; { @\FormatAq<Cl><03> }	{ chloride }
Cl _{2m}	= 2Cl	+ Min ; { @\FormatAq<Cl ₂ ><03> }	{ }
Cl _{0m}	= Cl + O	+ Min ; { @\FormatAq<ClO><03> }	{ }
ClOH _m	= H + O + Cl	+ Min ; { @\FormatAq<ClOH><03> }	{ }

{----- Br -----}

Br _m	= Br	+ Min ; { @\FormatAq <03> }	{ bromide }
Br _{2m}	= 2Br	+ Min ; { @\FormatAq<Br ₂ ><03> }	{ }
Br _{0m}	= Br + O	+ Min ; { @\FormatAq<BrO><03> }	{ }
BrOH _m	= H + O + Br	+ Min ; { @\FormatAq<BrOH><03> }	{ }
BrCl _{2m}	= Br + 2Cl	+ Min ; { @\FormatAq<BrCl ₂ ><03> }	{ }
Br ₂ Cl _m	= 2Br + Cl	+ Min ; { @\FormatAq<Br ₂ Cl><03> }	{ }

{----- I -----}

I _m	= I	+ Min ; { @\FormatAq<I><03> }	{ iodide }
IO _{2m}	= I + 2O	+ Min ; { @\FormatAq<IO ₂ ><03> }	{ }
IO _{3m}	= I + 3O	+ Min ; { @\FormatAq<IO ₃ ><03> }	{ iodate }
ICl _{2m}	= I + 2Cl	+ Min ; { @\FormatAq<ICl ₂ ><03> }	{ }
IBr _{2m}	= I + 2Br	+ Min ; { @\FormatAq<IBr ₂ ><03> }	{ }

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{----- S -----}

S03m_a03      = S + 30      + Min ; {@\FormatAq<SO_3^-><03>}      {}
S03mm_a03     = S + 30      + 2Min ; {@\FormatAq<SO_3^<2->><03>}    {sulfite}
S04m_a03      = S + 40      + Min ; {@\FormatAq<SO_4^-><03>}      {}
S04mm_a03     = S + 40      + 2Min ; {@\FormatAq<SO_4^<2->><03>}    {sulfate}
S05m_a03      = S + 50      + Min ; {@\FormatAq<SO_5^-><03>}      {}
HS03m_a03     = H + S + 30   + Min ; {@\FormatAq<HSO_3^-><03>}    {hydrogen sulfite}
HS04m_a03     = H + S + 40   + Min ; {@\FormatAq<HSO_4^-><03>}    {hydrogen sulfate}
HS05m_a03     = H + S + 50   + Min ; {@\FormatAq<HSO_5^-><03>}    {}
CH3SO3m_a03   = C + 3H + S + 30 + Min ; {@\FormatAq<CH_3SO_3^-><03>} {MSA anion}
CH2OHSO3m_a03 = C + 3H + S + 40 + Min ; {@\FormatAq<CH_2OHSO_3^-><03>} {}

{----- Hg -----}

Hgp_a03       = Hg          + Pls ; {@\FormatAq<Hg^+><03>}          {}
Hgpp_a03      = Hg          + 2Pls ; {@\FormatAq<Hg^<2+>><03>}      {}
HgOHp_a03     = Hg + O + H   + Pls ; {@\FormatAq<HgOH^+><03>}      {}
HgClp_a03     = Hg + Cl      + Pls ; {@\FormatAq<HgCl^+><03>}      {}
HgBrp_a03     = Hg + Br      + Pls ; {@\FormatAq<HgBr^+><03>}      {}
HgSO32mm_a03  = Hg + 2S + 60 + 2Min ; {@\FormatAq<Hg(SO_3)_2^<2->><03>} {}

{----- Fe -----}

Fepp_a03      = Fe          + 2Pls ; {@\FormatAq<Fe^<2+>><03>}      {Fe(II)}
Fe0pp_a03     = Fe + 0       + 2Pls ; {@\FormatAq<Fe0^<2+>><03>}    {Fe(II)}
FeOHp_a03     = Fe + 0 + H   + Pls ; {@\FormatAq<FeOH^+><03>}      {Fe(II)}
FeOH2p_a03    = Fe + 20 + 2H + Pls ; {@\FormatAq<Fe(OH)_2^+><03>}    {Fe(II)}
FeClp_a03     = Fe + Cl      + Pls ; {@\FormatAq<FeCl^+><03>}      {Fe(II)}
Feppp_a03     = Fe          + 3Pls ; {@\FormatAq<Fe^<3+>><03>}      {Fe(III)}
FeH0pp_a03    = Fe + 0 + H   + 2Pls ; {@\FormatAq<FeH0^<2+>><03>}   {Fe(III)}
FeH02pp_a03   = Fe + 20 + H + 2Pls ; {@\FormatAq<FeH0_2^<2+>><03>}   {Fe(III)}
FeOHpp_a03    = Fe + 0 + H   + 2Pls ; {@\FormatAq<FeOH^<2+>><03>}   {Fe(III)}
FeOH4m_a03    = Fe + 40 + 4H + Min ; {@\FormatAq<Fe(OH)_4^-><03>}    {Fe(III)}
FeOHH02p_a03  = Fe + 30 + 2H + Pls ; {@\FormatAq<Fe(OH)(HO_2)^+><03>} {Fe(III)}
FeClpp_a03    = Fe + Cl      + 2Pls ; {@\FormatAq<FeCl^<2+>><03>}    {Fe(III)}
FeCl2p_a03    = Fe + 2Cl     + Pls ; {@\FormatAq<FeCl_2^+><03>}     {Fe(III)}
FeBrpp_a03    = Fe + Br      + 2Pls ; {@\FormatAq<FeBr^<2+>><03>}    {Fe(III)}
FeBr2p_a03    = Fe + 2Br     + Pls ; {@\FormatAq<FeBr_2^+><03>}     {Fe(III)}
FeFpp_a03     = Fe + F       + 2Pls ; {@\FormatAq<FeF^<2+>><03>}     {Fe(III)}
FeF2p_a03     = Fe + 2F      + 2Pls ; {@\FormatAq<FeF_2^+><03>}      {Fe(III)}
FeS03p_a03    = Fe + 30 + S   + Pls ; {@\FormatAq<FeSO_3^+><03>}     {Fe(III)}
FeS04p_a03    = Fe + 40 + S   + Pls ; {@\FormatAq<FeSO_4^+><03>}     {Fe(III)}
FeS042m_a03   = Fe + 80 + 2S + Min ; {@\FormatAq<Fe(SO_4)_2^-><03>}   {Fe(III)}
FeOH2Fepppp_a03 = 2 Fe + 0 + H + 4Pls ; {@\FormatAq<Fe(OH)_2Fe^<4+>><03>} {Fe(III)}

{-----}
{----- dummies -----}
{-----}

D10_a03       = Ignore      ; {@\FormatAq<D_10><03>}      {}
Nap_a03       = Ignore      ; {@\FormatAq<Na^+><03>}      {dummy cation}
{-----}
{----- aerosol mode: 03 -----}
{-----}

{----- neutral species -----}

{----- 0 -----}

{----- H -----}

{----- N -----}
N203_a03      =          30 + 2N ; {@\FormatAq<N_20_3><03>}      {dinitrogen
trioxide}
N204_a03      =          40 + 2N ; {@\FormatAq<N_20_4><03>}      {dinitrogen
tetraoxide}

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{----- C -----}

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{1C}
CH2O2H2_a03    =  C + 4H + 20      ; {@\FormatAq<CH_2(OH)_2><03>}      {}
MMA_a03        =  C + 5H          + N ; {@\FormatAq<MMA><03>}          {methylamine}
NH2CH2_a03     =  C + 4H          + N ; {@\FormatAq<CH_2NH_2><03>}      {methylamine
radical}
HNCO_a03       =  C +   H +   0 + N ; {@\FormatAq<HNCO><03>}          {ioscyanic
acid}
H2NCHO_a03     =  C + 3H +   0 + N ; {@\FormatAq<H2NCHO><03>}          {formamide}
MMNNO2_a03     =  C + 2H + 20 + 2N ; {@\FormatAq<MMNNO2><03>}          {}
{methylnitramine}
MSIA_a03       =  C + 4H +   S + 20 ; {@\FormatAq<MSIA><03>}          {methyl
sulfinic acid}

{2C}
OXALAC_a03     =  IGNORE              ; {@\FormatAq<OXALAC><03>}          {oxalic acid,
2C + 2H + 40}
HCOCO2H_a03    =  2C + 2H + 30        ; {@\FormatAq<HCOCO_2H><03>}          {oxoethanoic
acid}
HOCH2CHO_a03   =  2C + 4H + 20        ; {@\FormatAq<HOCH_2CHO><03>}          {}
{glycolaldehyde}
HOCH2CO2H_a03  =  2C + 4H + 30        ; {@\FormatAq<HOCH_2CO_2H><03>}      {}
{hydroxyethanoic acid}
CH3CO3_a03     =  2C + 3H + 30        ; {@\FormatAq<CH_3COO_2><03>}          {peroxyacetyl
radical}
GLYOX_a03      =  2C + 2H + 20        ; {@\FormatAq<GLYOX><03>}          {CHOCHO =
glyoxal}
DMA_a03        =  2C + 7H          + N ; {@\FormatAq<DMA><03>}          {}
{dimethylamine}
MEA_a03        =  2C + 7H +   0 + N ; {@\FormatAq<MEA><03>}          {ethanolamine}
MEANNO_a03     =  2C + 6H + 20 + 2N ; {@\FormatAq<MEANNO><03>}          {N-nitroso
ethanolamine}
MEANNO2_a03    =  2C + 6H + 30 + 2N ; {@\FormatAq<MEANNO2><03>}          {N-nitro
ethanolamine}
NDMA_a03       =  2C + 6H +   0 + 2N ; {@\FormatAq<NDMA><03>}          {N-nitroso
dimethylamine}
DMNNO2_a03     =  2C + 6H + 20 + 2N ; {@\FormatAq<DMNNO2><03>}          {}
{dimethylnitramine}
CH3NHCH2_a03   =  2C + 6H +          N ; {@\FormatAq<CH_3NHCH_2><03>}      {methylamine
methyl radical}
CH3NHNHCH3_a03 =  2C + 8H +          2N ; {@\FormatAq<CH_3NHNHCH_3><03>}      {}
{dimethylhydrazine}
NH2C2H4NH2_a03 =  2C + 8H +          2N ; {@\FormatAq<NH_2CH_2CH_2NH_2><03>}  {}
{ethylenediamine}
NH2CH2CHOH_a03 =  2C + 6H +   0 + N ; {@\FormatAq<NH_2CH_2CHOH><03>}      {ethanolamine
radical}
H2NCOCH2OH_a03 =  2C + 5H + 20 + N ; {@\FormatAq<H2NCOCH2OH><03>}          {2-hydroxy
acetamide}
CH3NHCHO_a03   =  2C + 5H +   0 + N ; {@\FormatAq<CH_3NHCHO><03>}          {N-methyl
formamide}
CH3NCO_a03     =  2C + 3H +   0 + N ; {@\FormatAq<CH_3NCO><03>}          {methyl
isocyanic acid}
HPMTF_a03      =  2C + 4H + 30 + S ; {@\FormatAq<HPMTF><03>}          {hydroperoxyl
methyl thioformate}
HOOCH2SCO_a03  =  2C + 3H + 30 + S ; {@\FormatAq<HOOCH2SCO><03>}          {}

{3C}
MGLYOX_a03     =  3C + 4H + 20        ; {@\FormatAq<MGLYOX><03>}          {}
{methylglyoxal}
MGLYOAC_a03    =  3C + 4H + 30        ; {@\FormatAq<MGLYOAC><03>}          {}
{methylglyoxylic acid}
DOC_a03        =  IGNORE              ; {@\FormatAq<DOC><03>}          {dissolved
organic carbon DOC}
DOC0_a03       =  IGNORE              ; {@\FormatAq<DOC0><03>}          {oxidized DOC}
TMA_a03        =  3C + 9H          + N ; {@\FormatAq<TMA><03>}          {}
{trimethylamine}
DMNCH2_a03     =  3C + 8H          + N ; {@\FormatAq<(CH_3)_2NCH_2><03>}      {}
{dimethylamine methyl radical}

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DMNCHO_a03      = 3C + 7H + 0 + N ; {@\FormatAq<DMNCHO><03>}      {N,N-dimethyl
formamide}
MALONAC_a03     = IGNORE                      ; {@\FormatAq<MALONAC><03>}      {malonic
acid, 3C + 4H + 4O}

{4C}
DEA_a03         = 4C + 11H + 20 + N ; {@\FormatAq<DEA><03>}
{diethanolamine}
NDELA_a03       = 4C + 10H + 30 + 2N ; {@\FormatAq<NDELA><03>}      {N-nitroso
diethanolamine}
DEANN02_a03     = 4C + 10H + 40 + 2N ; {@\FormatAq<DEANN02><03>}      {N-nitro
diethanolamine}
DEAN_a03        = 4C + 10H + 20 + N ; {@\FormatAq<HOETNHCH_2CHOH><03>}
{diethanolamine radical}
SUCCAC_a03      = IGNORE                      ; {@\FormatAq<SUCCAC><03>}      {succinic
acid, 4C + 6H + 4O}

{5C}
GLUTARAC_a03    = IGNORE                      ; {@\FormatAq<GLUTARAC><03>}      {glutaric
acid, 5C + 8H + 4O}

{6C}
TEA_a03         = 6C + 15H + 30 + N ; {@\FormatAq<TEA><03>}
{triethanolamine}
DENCH2CHOH_a03  = 6C + 14H + 30 + N ; {@\FormatAq<DENCH_2CHOH><03>}
{triethanolamine radical}
ADIPAC_a03      = IGNORE                      ; {@\FormatAq<ADIPAC><03>}      {adipic acid,
6C + 10H + 4O}

{----- ions -----}

{----- O -----}

{----- H -----}

{----- N -----}

{----- C -----}

{1C}
MMAp_a03        = C + 6H + N + Pls ; {@\FormatAq<MMA^+><03>}
{methylaminium}
MMNp_a03        = C + 5H + N + Pls ; {@\FormatAq<CH_3NH_2^+><03>}
{methylamine N-radical cation}
NH2CH2p_a03     = C + 4H + N + Pls ; {@\FormatAq<CH_2NH_2^+><03>}
{iminium}
NH3CH2p_a03     = C + 5H + N + Pls ; {@\FormatAq<CH_2NH_3^+><03>}
{methylaminium radical}
NC0m_a03        = C + 0 + N + Min ; {@\FormatAq<NC0^-><03>}
{isocyanate}

{2C}
HC204m_a03      = IGNORE + Min ; {@\FormatAq<HC_20_4^-><03>}
{hydrogen oxalate, 2C + H + 4O}
C204mm_a03      = IGNORE + 2Min ; {@\FormatAq<C_20_4^<2->><03>}
{oxalate, 2C + 4O}
HCOCO0m_a03     = 2C + H + 30 + Min ; {@\FormatAq<HCOCO0^><03>}      {}
MEAp_a03        = 2C + 8H + 0 + N + Pls ; {@\FormatAq<MEA^+><03>}
{ethanolaminium}
DMAp_a03        = 2C + 8H + N + Pls ; {@\FormatAq<DMA^+><03>}
{dimethylaminium}
DMNp_a03        = 2C + 7H + N + Pls ; {@\FormatAq<(CH_3)_2NH^+><03>}
{dimethylamine N-radical cation}
CH3NHCH2p_a03   = 2C + 6H + N + Pls ; {@\FormatAq<CH_3NH^+CH_2><03>}
{methyl iminium}
CH3NH2CH2p_a03  = 2C + 7H + N + Pls ; {@\FormatAq<CH_3NH_2^+CH_2><03>}
{dimethylaminium radical}

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MENp_a03      = 2C + 7H + 0 + N + Pls ; {@\FormatAq<HOCH_2CH_2NH_2^+><03>}
{ethanolamine N-radical cation}
NH3CH2CHOHp_a03 = 2C + 7H + 0 + N + Pls ; {@\FormatAq<HOCHCH_2NH_3^+><03>}
{ethanolaminium radical}

{3C}
CH3COCOOm_a03 = 3C + 3H + 30 + Min ; {@\FormatAq<CH_3COCOO^-><03>}
{methylglyoxalate}
TMAp_a03      = 3C + 10H + N + Pls ; {@\FormatAq<TMA^+><03>}
{trimethylaminium}
TMNp_a03      = 3C + 9H + N + Pls ; {@\FormatAq<(CH_3)_3N^+><03>}
{trimethylamine N-radical cation}
DMNCH2p_a03   = 3C + 8H + N + Pls ; {@\FormatAq<(CH_3)_2N^+CH_2><03>}
{dimethyl iminium}
DMNHCH2p_a03  = 3C + 9H + N + Pls ; {@\FormatAq<(CH_3)_2NH^+CH_2><03>}
{trimethylaminium radical}

{4C}
DEAp_a03      = 4C + 12H + 20 + N + Pls ; {@\FormatAq<DEA^+><03>}
{diethanolaminium}
DENp_a03      = 4C + 13H + 20 + N + Pls ; {@\FormatAq<(HOET)_2NH^+><03>}
{diethanolamine N-radical cation}
DENHp_a03     = 4C + 12H + 20 + N + Pls ; {@\FormatAq<HOETNH_2CH_2CHOH^+><03>}
{diethanolaminium radical}
C2H5C2O4m_a03 = IGNORE + Min ; {@\FormatAq<CH_2CH_2HC_2O_4^-><03>}
{hydrogen succinate, 4C + 5H + 40}
C2H4C2O4mm_a03 = IGNORE + 2Min ; {@\FormatAq<CH_2CH_2C_2O_4^<2->><03>}
{succinate, 4C + 4H + 40}

{6C}
TEAp_a03      = 6C + 16H + 30 + N + Pls ; {@\FormatAq<TEA^+><03>}
{triethanolaminium}
TENp_a03      = 6C + 15H + 30 + N + Pls ; {@\FormatAq<(HOET)_3N^+><03>}
{triethanolamine N-radical cation}
DENIMp_a03    = 6C + 15H + 30 + N + Pls ; {@\FormatAq<(HOET)_2N^+CH_2CH_2OH><03>}
{diethanol iminium}
TENHp_a03     = 6C + 15H + 30 + N + Pls ; {@\FormatAq<(HOET)_2NH^+CH_2CHOH><03>}
{triethanolaminium radical}

{-----M-----}
{**** END: aerosol species (phase 3) from aqueous.spc ****}
{SETFIX H2O_a* is done via xmecca}
#SETFIX H2O_a01;
#SETFIX H2O_a02;
#SETFIX H2O_a03;

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