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{created automatically by xmecca, DO NOT EDIT!}
{xmecca was run on 2021-03-18 at 18:51:49 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>}

{------------------------------------------------------------------------------}

{ 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 ROOH, all peroxy radicals are called RO2          }
{ - 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 sytax follows after the "@" sign.         }

{------------------------------------------------------------------------------}

#DEFVAR

{------------------------------------------------------------------------------}
{---------------------------------- gas phase ---------------------------------}
{------------------------------------------------------------------------------}

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

O1D             =  O                  ; {@O(^1D)}            {O singlet D}
O3P             =  O                  ; {@O(^3P)}            {O triplet P}
O2              = 2O                  ; {@O_2}               {oxygen}
O3              = 3O                  ; {@O_3}               {ozone}

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

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}

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

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}
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N2O5            =      5O + 2N         ; {@N_2O_5}            {dinitrogen
pentoxide}
HONO            =  H + 2O +  N         ; {@HONO}              {nitrous acid}
HNO3            =  H + 3O +  N         ; {@HNO_3}             {nitric acid}
HNO4            =  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)}
CH2OO           =   C +  2H +  2O      ; {@CH_2OO}            {MCM: carbonyl oxide
- stabilized Criegee Intermediate}
CH2OOA          =   C +  2H +  2O      ; {@CH_2OO^*}          {MCM: carbonyl oxide
- excited Criegee Intermediate}
CH3             =   C +  3H            ; {@CH_3}              {methyl radical}
CH3O            =   C +  3H +   O      ; {@CH_3O}             {MCM: methoxy
radical}
CH3O2           =   C +  3H +  2O      ; {@CH_3O_2}           {MCM: methylperoxy
radical}
CH3OH           =   C +  4H +   O      ; {@CH_3OH}            {MCM: methanol}
CH3OOH          =   C +  4H +  2O      ; {@CH_3OOH}           {MCM: methyl
peroxide}
CH4             =   C +  4H            ; {@CH_4}              {MCM: methane}
CO              =   C       +   O      ; {@CO}                {carbon monoxide}
CO2             =   C       +  2O      ; {@CO_2}              {carbon dioxide}
HCHO            =   C +  2H +   O      ; {@HCHO}              {MCM: methanal =
formaldehyde}
HCOOH           =   C +  2H +  2O      ; {@HCOOH}             {MCM: formic acid}
HOCH2O2         =   C +  3H +  3O      ; {@HOCH_2O_2}         {hydroxy methyl
peroxy radical}
HOCH2OH         =   C +  4H +  2O      ; {@HOCH_2OH}          {dyhydroxy methane}
HOCH2OOH        =   C +  4H +  3O      ; {@HOCH_2OOH}         {hydroxy methyl
hydroperoxide}
{1C (CHON)}
CH3NO3          =   C +  3H +  3O +  N ; {@CH_3ONO_2}         {MCM: methylnitrate}
CH3O2NO2        =   C +  3H +  4O +  N ; {@CH_3O_2NO_2}       {MCM: peroxy
methylnitrate}
CH3ONO          =   C +  3H +  2O +  N ; {@CH_3ONO}           {methylnitrite}
CN              =   C             +  N ; {@CN}                {}
HCN             =   C +   H       +  N ; {@HCN}               {}
HOCH2O2NO2      =   C +  3H +  5O +  N ; {@HOCH_2O_2NO_2}     {hydroxy methyl
peroxy nitrate}
NCO             =   C       +   O +  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}
C2H5O2          =  2C +  5H +  2O      ; {@C_2H_5O_2}         {MCM: ethylperoxy
radical}
C2H5OH          =  2C +  6H +   O      ; {@C_2H_5OH}          {MCM: ethanol}
C2H5OOH         =  2C +  6H +  2O      ; {@C_2H_5OOH}         {MCM: ethyl hydro
peroxide}
C2H6            =  2C +  6H            ; {@C_2H_6}            {MCM: ethane}
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CH2CHOH         =  2C +  4H +   O      ; {@CH_2CHOH}          {vinyl alcohol}
CH2CO           =  2C +  2H +   O      ; {@CH2CO}             {ketene}
CH3CHO          =  2C +  4H +   O      ; {@CH_3CHO}           {MCM: acetaldehyde}
CH3CHOHO2       =  2C +  5H +  3O      ; {@CH3CHOHO2}         {}
CH3CHOHOOH      =  2C +  6H +  3O      ; {@CH3CHOHOOH}        {}
CH3CO           =  2C +  3H +  2O      ; {@CH_3C(O)}          {acetyl radical}
CH3CO2H         =  2C +  4H +  2O      ; {@CH_3COOH}          {MCM: acetic acid}
CH3CO3          =  2C +  3H +  3O      ; {@CH_3C(O)OO}        {MCM: peroxy acetyl
radical}
CH3CO3H         =  2C +  4H +  3O      ; {@CH_3C(O)OOH}       {MCM: peroxy acetic
acid}
ETHGLY          =  2C +  6H +  2O      ; {@ETHGLY}            {MCM: HOCH2CH2OH}
GLYOX           =  2C +  2H +  2O      ; {@GLYOX}             {MCM: CHOCHO =
glyoxal}
HCOCH2O2        =  2C +  3H +  3O      ; {@HCOCH_2O_2}        {MCM}
HCOCO           =  2C +   H +  2O      ; {@HCOCO}             {MOM}
HCOCO2H         =  2C +  2H +  3O      ; {@HCOCO_2H}          {MCM: oxoethanoic
acid}
HCOCO3          =  2C +   H +  4O      ; {@HCOCO_3}           {MCM}
HCOCO3H         =  2C +  2H +  4O      ; {@HCOCO_3H}          {MCM}
HOCH2CH2O       =  2C +  5H +  2O      ; {@HOCH_2CH_2O}       {MCM: (2-
hydroxyethyl)oxidanyl}
HOCH2CH2O2      =  2C +  5H +  3O      ; {@HOCH_2CH_2O_2}     {MCM: (2-
hydroxyethyl)dioxidanyl}
HOCH2CHO        =  2C +  4H +  2O      ; {@HOCH_2CHO}         {MCM: glycolaldehyde}
HOCH2CO         =  2C +  3H +  2O      ; {@HOCH2CO}           {}
HOCH2CO2H       =  2C +  4H +  3O      ; {@HOCH_2CO_2H}       {MCM: hydroxyethanoic
acid}
HOCH2CO3        =  2C +  3H +  4O      ; {@HOCH_2CO_3}        {MCM}
HOCH2CO3H       =  2C +  4H +  4O      ; {@HOCH_2CO_3H}       {MCM}
HOCHCHO         =  2C +  3H +  2O      ; {@HOCHCHO}           {}
HOOCH2CHO       =  2C +  4H +  3O      ; {@HOOCH2CHO}         {}
HOOCH2CO2H      =  2C +  4H +  4O      ; {@HOOCH2CO2H}        {}
HOOCH2CO3       =  2C +  3H +  5O      ; {@HOOCH_2CO_3}       {}
HOOCH2CO3H      =  2C +  4H +  5O      ; {@HOOCH2CO3H}        {}
HYETHO2H        =  2C +  6H +  3O      ; {@HYETHO2H}          {MCM: HOCH2CH2OOH}
{2C (CHON)}
C2H5NO3         =  2C +  5H +  3O +  N ; {@C_2H_5ONO_2}       {MCM: ethyl nitrate}
C2H5O2NO2       =  2C +  5H +  4O +  N ; {@C_2H_5O_2NO_2}     {ethyl peroxy
nitrate}
CH3CN           =  2C +  3H       +  N ; {@CH_3CN}           {acetonitrile}
ETHOHNO3        =  2C +  5H +  4O +  N ; {@ETHOHNO3}         {MCM: HOCH2CH2ONO2}
NCCH2O2         =  2C +  2H +  2O +  N ; {@NCCH_2O_2}        {}
NO3CH2CHO       =  2C +  3H +  4O +  N ; {@NO_3CH2CHO}       {MCM}
NO3CH2CO3       =  2C +  2H +  6O +  N ; {@NO_3CH2CO_3}      {MCM}
NO3CH2PAN       =  2C +  2H +  8O + 2N ; {@NO_3CH2CHO}       {MCM}
PAN             =  2C +  3H +  5O +  N ; {@PAN}              {MCM: CH3C(O)OONO2 =
peroxyacetylnitrate}
PHAN            =  2C +  3H +  6O +  N ; {@PHAN}             {MCM: HOCH2C(O)OONO2}
{3C (CHO)}
ACETOL          =  3C +  6H +  2O      ; {@CH_3COCH_2OH}      {MCM: HO-CH2-CO-CH3 =
hydroxy acetone}
ALCOCH2OOH      =  3C +  4H +  4O      ; {@HCOCOCH_2OOH}      {MCM}
C2H5CHO         =  3C +  6H +   O      ; {@C_2H_5CHO}         {MCM: propanal}
PROPACID        =  3C +  6H +  2O      ; {@C_2H_5CO_2H}       {MCM}
C2H5CO3         =  3C +  5H +  3O      ; {@C_2H_5CO_3}        {MCM}
PERPROACID      =  3C +  6H +  3O      ; {@C_2H_5CO_3H}       {MCM}
C33CO           =  3C +  2H +  3O      ; {@HCOCOCHO}          {MCM}
C3H6            =  3C +  6H            ; {@C_3H_6}            {MCM: propene}
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C3H8            =  3C +  8H           ; {@C_3H_8}            {MCM: propane}
CH3CHCO         =  3C +  4H +   O     ; {@CH3CHCO}           {CH3CHCO}
CH3COCH2O2      =  3C +  5H +  3O     ; {@CH_3COCH_2O_2}     {MCM: peroxyradical
from acetone}
CH3COCH3        =  3C +  6H +   O     ; {@CH_3COCH_3}        {MCM: acetone}
CH3COCO2H       =  3C +  4H +  3O     ; {@CH_3COCO_2H}       {MCM: pyruvic acid}
CH3COCO3        =  3C +  3H +  4O     ; {@CH_3COCO_3}        {MCM}
CH3COCO3H       =  3C +  4H +  4O     ; {@CH_3COCO_3H}       {MCM}
CHOCOCH2O2      =  3C +  3H +  4O     ; {@HCOCOCH_2O_2}      {MCM}
HCOCH2CHO       =  3C +  4H +  3O     ; {@HCOCH2CHO}         {MCM}
HCOCH2CO2H      =  3C +  4H +  4O     ; {@HCOCH2CO2H}        {MCM}
HCOCH2CO3       =  3C +  3H +  5O     ; {@HCOCH2CO3}         {MCM}
HCOCH2CO3H      =  3C +  4H +  5O     ; {@HCOCH2CO3H}        {MCM}
HCOCOCH2OOH     =  3C +  4H +  4O     ; {@HCOCOCH_2OOH}      {}
HOC2H4CO2H      =  3C +  6H +  3O     ; {@HOC2H4CO2H}        {MCM: 3-
hydroxypropanoic acid}
HOC2H4CO3       =  3C +  5H +  4O     ; {@HOC_2H_4CO_3}      {MCM}
HOC2H4CO3H      =  3C +  6H +  4O     ; {@HOC2H4CO3H}        {MCM}
HOCH2COCH2O2    =  3C +  5H +  4O     ; {@HOCH2COCH2O2}      {}
HOCH2COCH2OOH   =  3C +  6H +  4O     ; {@HOCH2COCH2OOH}     {}
HOCH2COCHO      =  3C +  4H +  3O     ; {@HOCH2COCHO}        {MCM:
hydroxypyruvaldehyde}
HYPERACET       =  3C +  6H +  3O     ; {@CH_3COCH_2O_2H}    {MCM: hydroperoxide
from CH3COCH2O2}
HYPROPO2        =  3C +  7H +  3O     ; {@HYPROPO2}          {MCM: CH3CH(O2)CH2OH}
HYPROPO2H       =  3C +  8H +  3O     ; {@HYPROPO2H}         {MCM:
CH3CH(OOH)CH2OH}
IC3H7O2         =  3C +  7H +  2O     ; {@iC_3H_7O_2}        {MCM: isopropylperoxy
radical}
IC3H7OOH        =  3C +  8H +  2O     ; {@iC_3H_7OOH}        {MCM: isopropyl hydro
peroxide}
IPROPOL         =  3C +  8H +   O     ; {@IPROPOL}           {MCM: isopropylic
alcohol}
MGLYOX          =  3C +  4H +  2O     ; {@MGLYOX}            {MCM: CH3COCHO =
methylglyoxal}
NC3H7O2         =  3C +  7H +  2O     ; {@C_3H_7O_2}         {MCM: propylperoxy
radical}
NC3H7OOH        =  3C +  8H +  2O     ; {@C_3H_7OOH}         {MCM: propyl hydro
peroxide}
NPROPOL         =  3C +  8H +   O     ; {@NPROPOL}           {MCM: n-propylic
alcohol}
PROPENOL        =  3C +  6H +   O     ; {@CH_2CHCH_2OH}      {}
{3C (CHO) aromatics}
C32OH13CO       =  3C +  4H +  3O     ; {@C32OH13CO}         {MCM:
hydroxymalonaldehyde}
C3DIALO2        =  3C +  3H +  4O     ; {@C3DIALO2}          {MCM}
C3DIALOOH       =  3C +  4H +  4O     ; {@C3DIALOOH}         {MCM}
HCOCOHCO3       =  3C +  3H +  5O     ; {@HCOCOHCO3}         {MCM}
HCOCOHCO3H      =  3C +  4H +  5O     ; {@HCOCOHCO3H}        {MCM}
METACETHO       =  3C +  4H +  3O     ; {@METACETHO}         {MCM: acetic formic
anhydride}
{3C (CHON)}
C3PAN1          =  3C +  5H +  6O +  N ; {@C_3PAN1}           {MCM}
C3PAN2          =  3C +  3H +  6O +  N ; {@C_3PAN2}           {MCM}
CH3COCH2O2NO2   =  3C +  5H +  5O +  N ; {@CH_3COCH_2OONO_2}  {CH3-C(O)-CH2-OONO2}
IC3H7NO3        =  3C +  7H +  3O +  N ; {@iC_3H_7ONO_2}      {MCM: isopropyl
nitrate}
NC3H7NO3        =  3C +  7H +  3O +  N ; {@C_3H_7ONO_2}       {MCM: propyl nitrate}
NOA             =  3C +  5H +  4O +  N ; {@NOA}               {MCM: CH3-CO-CH2ONO2
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= nitro-oxy-acetone}
PPN             =  3C +  5H +  5O +  N ; {@PPN}               {MCM:
CH3CH2C(O)OONO2}
PR2O2HNO3       =  3C +  7H +  5O +  N ; {@PR2O2HNO3}         {MCM: CH3-CH(OOH)-
CH2ONO2}
PRONO3BO2       =  3C +  6H +  5O +  N ; {@PRONO3BO2}         {MCM: CH3-CH(O2)-
CH2ONO2}
PROPOLNO3       =  3C +  7H +  4O +  N ; {@PROPOLNO3}         {MCM: HOCH2-
CH(CH3)ONO2)}
{3C (CHON) aromatics}
HCOCOHPAN       =  3C +  3H +  7O +  N ; {@HCOCOHPAN}         {MCM}
{4C (CHO)}
BIACET          =  4C +  6H +  2O      ; {@BIACET}            {MCM: CH3-CO-CO-CH3}
BIACETO2        =  4C +  5H +  4O      ; {@CH_3COCOCH_2O_2}   {MCM}
BIACETOH        =  4C +  6H +  3O      ; {@BIACETOH}          {MCM: CH3-CO-CO-
CH2OH}
BIACETOOH       =  4C +  6H +  4O      ; {@CH_3COCOCH_2OOH}   {MCM}
BUT1ENE         =  4C +  8H            ; {@BUT1ENE}           {MCM}
BUT2OLO         =  4C +  8H +  3O      ; {@BUT2OLO}           {MCM}
BUT2OLO2        =  4C +  9H +  2O      ; {@BUT2OLO2}          {MCM}
BUT2OLOOH       =  4C + 10H +  3O      ; {@BUT2OLOOH}         {MCM}
BUTENOL         =  4C +  8H +   O      ; {@BUTENOL}           {CH3CH2CHCHOH}
C312COCO3       =  4C +  3H +  5O      ; {@C312COCO3}         {MCM}
C312COCO3H      =  4C +  4H +  5O      ; {@C312COCO3H}        {MCM}
C3H7CHO         =  4C +  8H +   O      ; {@C_3H_7CHO}         {MCM: n-butanal}
C413COOOH       =  4C +  6H +  4O      ; {@C413COOOH}         {MCM}
C44O2           =  4C +  5H +  5O      ; {@C44O2}             {MCM}
C44OOH          =  4C +  6H +  5O      ; {@C44OOH}            {MCM}
C4CODIAL        =  4C +  4H +  3O      ; {@C4CODIAL}          {MCM}
CBUT2ENE        =  4C +  8H            ; {@CBUT2ENE}          {MCM}
CH3COCHCO       =  4C +  4H +  2O      ; {@CH_3COCHCO}        {}
CH3COCHO2CHO    =  4C +  5H +  4O      ; {@CH_3COCHO_2CHO}    {}
CH3COCOCO2H     =  4C +  6H +  4O      ; {@CH3COCOCO2H}       {}
CH3COOHCHCHO    =  4C +  6H +  3O      ; {@CH_3COOHCHCHO}     {}
CHOC3COO2       =  4C +  5H +  4O      ; {@CHOC3COO2}         {MCM}
CO23C3CHO       =  4C +  4H +  3O      ; {@CH_3COCOCHO}       {MCM}
CO2C3CHO        =  4C +  6H +  2O      ; {@CO2C3CHO}          {MCM: CH3COCH2CHO}
CO2H3CHO        =  4C +  5H +  3O      ; {@CO2H3CHO}          {MCM: CH3-CO-CH(OH)-
CHO}
CO2H3CO2H       =  4C +  6H +  5O      ; {@CO2H3CO2H}         {}
CO2H3CO3        =  4C +  5H +  5O      ; {@CO2H3CO3}          {MCM: CH3-CO-CH(OH)-
C(O)O2}
CO2H3CO3H       =  4C +  6H +  5O      ; {@CO2H3CO3H}         {MCM: CH3-CO-CH(OH)-
C(O)OOH}
EZCH3CO2CHCHO   =  4C +  5H +  3O      ; {@EZCH3CO2CHCHO}     {}
EZCHOCCH3CHO2   =  4C +  5H +  3O      ; {@EZCHOCCH3CHO2}     {}
HCOCCH3CHOOH    =  4C +  6H +  3O      ; {@HCOCCH_3CHOOH}     {}
HCOCCH3CO       =  4C +  4H +  2O      ; {@HCOCCH_3CO}        {}
HCOCO2CH3CHO    =  4C +  5H +  4O      ; {@HCOCO_2CH_3CHO}    {}
HMAC            =  4C +  6H +  2O      ; {@HMAC}              {MCM: HCOC(CH3)CHOH}
HO12CO3C4       =  4C +  8H +  3O      ; {@HO12CO3C4}         {MCM: CH3-CO-CH(OH)-
CH2OH}
HVMK            =  4C +  6H +  2O      ; {@HVMK}              {MCM: CH3COCHCHOH =
hydroxy vinyl methyl ketone}
IBUTALOH        =  4C +  8H +  2O      ; {@IBUTALOH}          {MCM}
IBUTDIAL        =  4C +  6H +  2O      ; {@IBUTDIAL}          {MCM: HCOC(CH3)CHO}
IBUTOLBO2       =  4C +  9H +  2O      ; {@IBUTOLBO2}         {MCM}
IBUTOLBOOH      =  4C + 10H +  3O      ; {@IBUTOLBOOH}        {}
IC4H10          =  4C + 10H            ; {@iC_4H_<10>}        {MCM: (CH3)3-CH = i-
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butane}
IC4H9O2         =  4C +  9H +  2O      ; {@IC_4H_9O_2}        {MCM: (CH3)2-CHCH2O2
IC4H9O2}
IC4H9OOH        =  4C + 10H +  2O      ; {@IC_4H_9OOH}        {MCM: (CH3)2-CHCH2OOH
MCM: IC4H9OOH}
IPRCHO          =  4C +  8H +   O      ; {@IPRCHO}            {MCM: (CH3)2CHCHO MCM
: methylpropanal}
IPRCO3          =  4C +  7H +  3O      ; {@IPRCO3}            {MCM: (CH3)2CHCO3}
IPRHOCO2H       =  4C +  8H +  3O      ; {@IPRHOCO2H}         {MCM}
IPRHOCO3        =  4C +  7H +  4O      ; {@IPRHOCO3}          {MCM}
IPRHOCO3H       =  4C +  8H +  4O      ; {@IPRHOCO3H}         {MCM}
MACO2           =  4C +  5H +  2O      ; {@MACO2}             {}
MACO2H          =  4C +  6H +  2O      ; {@MACO2H}            {MCM: CH2=C(CH3)COOH
= methacrylic acid}
MACO3           =  4C +  5H +  3O      ; {@MACO3}             {MCM:
CH2=C(CH3)C(O)O2}
MACO3H          =  4C +  6H +  3O      ; {@MACO3H}            {MCM:
CH2=C(CH3)C(O)OOH}
MACR            =  4C +  6H +   O      ; {@MACR}              {MCM: CH2=C(CH3)CHO =
methacrolein}
MACRO           =  4C +  7H +  3O      ; {@MACRO}             {MCM}
MACRO2          =  4C +  7H +  4O      ; {@MACRO2}            {MCM: HOCH2C(OO)
(CH3)CHO}
MACROH          =  4C +  8H +  3O      ; {@MACROH}            {MCM: HOCH2C(OH)
(CH3)CHO}
MACROOH         =  4C +  8H +  4O      ; {@MACROOH}           {MCM: HOCH2C(OOH)
(CH3)CHO}
MBOOO           =  4C +  8H +  3O      ; {@MBOOO}             {MCM}
MEK             =  4C +  8H +   O      ; {@MEK}               {MCM: CH3-CO-CH2-CH3
= methyl ethyl ketone}
MEPROPENE       =  4C +  8H            ; {@MEPROPENE}         {MCM}
MPROPENOL       =  4C +  8H +   O      ; {@MPROPENOL}         {(CH3)2CCHOH
methylpropenol}
MVK             =  4C +  6H +   O      ; {@MVK}               {MCM: CH3-CO-CH=CH2 =
methyl vinyl ketone}
NC4H10          =  4C + 10H            ; {@C_4H_<10>}         {MCM: CH3-CH2-CH2-CH3
= n-butane}
PERIBUACID      =  4C +  8H +  3O      ; {@PERIBUACID}        {MCM: (CH3)2CHCO3H}
TBUT2ENE        =  4C +  8H            ; {@TBUT2ENE}          {MCM}
TC4H9O2         =  4C +  9H +  2O      ; {@TC_4H_9O_2}        {MCM: (CH3)3-CO2}
TC4H9OOH        =  4C + 10H +  2O      ; {@TC_4H_9OOH}        {MCM: (CH3)3-COOH}
{4C (CHO) aromatics}
BZFUCO          =  4C +  4H +  4O      ; {@BZFUCO}            {MCM}
BZFUO2          =  4C +  5H +  3O      ; {@BZFUO2}            {MCM}
BZFUONE         =  4C +  4H +  2O      ; {@BZFUONE}           {MCM: 2(5H)-furanone}
BZFUOOH         =  4C +  6H +  5O      ; {@BZFUOOH}           {MCM}
CO14O3CHO       =  4C +  4H +  4O      ; {@CO14O3CHO}         {MCM}
CO14O3CO2H      =  4C +  4H +  5O      ; {@CO14O3CO2H}        {MCM}
CO2C4DIAL       =  4C +  2H +  4O      ; {@CO2C4DIAL}         {MCM: 2,3-
dioxosuccinaldehyde}
EPXC4DIAL       =  4C +  4H +  3O      ; {@EPXC4DIAL}         {MCM}
EPXDLCO2H       =  4C +  4H +  4O      ; {@EPXDLCO2H}         {MCM}
EPXDLCO3        =  4C +  3H +  5O      ; {@EPXDLCO3}          {MCM}
EPXDLCO3H       =  4C +  4H +  5O      ; {@EPXDLCO3H}         {MCM}
HOCOC4DIAL      =  4C +  4H +  4O      ; {@HOCOC4DIAL}        {MCM: 2-hydroxy-3-
oxosuccinaldehyde}
MALANHY         =  4C +  2H +  3O      ; {@MALANHY}           {MCM: maleic
anhydride}
MALANHYO2       =  4C +  3H +  6O      ; {@MALANHYO2}         {MCM}
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MALANHYOOH      =  4C +  4H +  6O      ; {@MALANHYOOH}        {MCM}
MALDALCO2H      =  4C +  4H +  3O      ; {@MALDALCO2H}        {MCM: 4-oxo-2-
butenoic acid}
MALDALCO3H      =  4C +  4H +  4O      ; {@MALDALCO3H}        {MCM}
MALDIAL         =  4C +  4H +  2O      ; {@MALDIAL}           {MCM: 2-butenedial}
MALDIALCO3      =  4C +  3H +  4O      ; {@MALDIALCO3}        {MCM}
MALDIALO2       =  4C +  5H +  5O      ; {@MALDIALO2}         {MCM}
MALDIALOOH      =  4C +  6H +  5O      ; {@MALDIALOOH}        {MCM}
MALNHYOHCO      =  4C +  2H +  5O      ; {@MALNHYOHCO}        {MCM}
MECOACEOOH      =  4C +  6H +  5O      ; {@MECOACEOOH}        {MCM}
MECOACETO2      =  4C +  5H +  5O      ; {@MECOACETO2}        {MCM}
{4C (CHON)}
BUT2OLNO3       =  4C +  9H +  5O +  N ; {@BUT2OLNO3}         {MCM}
C312COPAN       =  4C +  3H +  7O +  N ; {@C312COPAN}         {MCM}
C4PAN5          =  4C +  7H +  6O +  N ; {@C4PAN5}            {MCM}
IBUTOLBNO3      =  4C +  9H +  4O +  N ; {@IBUTOLBNO3}        {MCM}
IC4H9NO3        =  4C +  9H +  3O +  N ; {@IC4H9NO3}          {MCM}
MACRNO3         =  4C +  7H +  5O +  N ; {@MACRNO3}           {MCM}
MPAN            =  4C +  5H +  5O +  N ; {@MPAN}              {MCM:
CH2=C(CH3)C(O)OONO2 = peroxymethacryloyl nitrate = peroxymethacrylic nitric
anhydride}
MVKNO3          =  4C +  7H +  5O +  N ; {@MVKNO3}           {MCM}
PIPN            =  4C +  7H +  5O +  N ; {@PIPN}             {MCM: (CH3)2CHCO3}
TC4H9NO3        =  4C +  9H +  3O +  N ; {@TC4H9NO3}         {MCM}
{4C (CHON) aromatics}
EPXDLPAN        =  4C +  3H +  7O +  N ; {@EPXDLPAN}         {MCM}
MALDIALPAN      =  4C +  3H +  6O +  N ; {@MALDIALPAN}       {MCM}
NBZFUO2         =  4C +  4H +  7O +  N ; {@NBZFUO2}          {MCM}
NBZFUONE        =  4C +  3H +  6O +  N ; {@NBZFUONE}         {MCM}
NBZFUOOH        =  4C +  5H +  7O +  N ; {@NBZFUOOH}         {MCM}
NC4DCO2H        =  4C +  3H +  5O +  N ; {@NC4DCO2H}         {MCM}
{4C (CHO) (lumped)}
LBUT1ENO2       =  4C +  9H +  2O      ; {@LBUT1ENO2}         {HO3C4O2 + NBUTOLAO2}
LBUT1ENOOH      =  4C + 10H +  3O      ; {@LBUT1ENOOH}        {HO3C4OOH +
NBUTOLAOOH}
LC4H9O2         =  4C +  9H +  2O      ; {@LC_4H_9O_2}        {CH3-CH2-CH(O2)-CH3 +
CH3-CH2-CH2-CH2O2 = NC4H9O2 + SC4H9O2}
LC4H9OOH        =  4C + 10H +  2O      ; {@LC_4H_9OOH}        {CH3-CH2-CH(OOH)-CH3
+ CH3-CH2-CH2-CH2OOH = NC4H9OOH + SC4H9OOH}
LHMVKABO2       =  4C +  7H +  4O      ; {@LHMVKABO2}         {HOCH2-CH(O2)-CO-CH3
+ CH2(O2)-CH(OH)-CO-CH3}
LHMVKABOOH      =  4C +  8H +  4O      ; {@LHMVKABOOH}        {HOCH2-CH(OOH)-CO-CH3
+ CH2(OOH)-CH(OH)-CO-CH3}
LMEKO2          =  4C +  7H +  3O      ; {@LMEKO2}            {CH3-CO-CH2-CH2-OO +
CH3-CO-CH(O2)-CH3}
LMEKOOH         =  4C +  8H +  3O      ; {@LMEKOOH}           {CH3-CO-CH2-CH2-OOH +
CH3-CO-CH(OOH)-CH3}
{4C (CHON) (lumped)}
LBUT1ENNO3      =  4C +  9H +  5O +  N ; {@LBUT1ENNO3}        {HO3C4NO3 +
NBUTOLANO3}
LC4H9NO3        =  4C +  9H +  3O +  N ; {@LC4H9NO3}          {NC4H9NO3 + SC4H9NO3}
LMEKNO3         =  4C +  7H +  5O +  N ; {@LMEKNO3}           {CH3-CO-CH2-CH2-ONO2
+ CH3-CO-CH(ONO2)-CH3}
{5C (CHO)}
C1ODC2O2C4OD    =  5C +  7H +  4O      ; {@C1ODC2O2C4OD}      {}
C1ODC2O2C4OOH   =  5C +  9H +  5O      ; {@C1ODC2O2C4OOH}     {}
C1ODC2OOHC4OD   =  5C +  8H +  4O      ; {@C1ODC2OOHC4OD}     {}
C1ODC3O2C4OOH   =  5C +  9H +  5O      ; {@C1ODC3O2C4OOH}     {}
C1OOHC2O2C4OD   =  5C +  9H +  5O      ; {@C1OOHC2O2C4OD}     {}
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C1OOHC2OOHC4OD  =  5C + 10H +  5O      ; {@C1OOHC2OOHC4OD}    {}
C1OOHC3O2C4OD   =  5C +  9H +  5O      ; {@C1OOHC3O2C4OD}     {}
C4MDIAL         =  5C +  6H +  2O      ; {@C4MDIAL}           {MCM: 2-methyl-
butenedial}
C511O2          =  5C +  7H +  4O      ; {@C511O2}            {MCM}
C511OOH         =  5C +  8H +  4O      ; {@C511OOH}           {MCM}
C512O2          =  5C +  7H +  4O      ; {@C512O2}            {MCM}
C512OOH         =  5C +  8H +  4O      ; {@C512OOH}           {MCM}
C513CO          =  5C +  6H +  4O      ; {@C513CO}            {MCM}
C513O2          =  5C +  7H +  5O      ; {@C513O2}            {MCM}
C513OOH         =  5C +  8H +  5O      ; {@C513OOH}           {MCM}
C514O2          =  5C +  7H +  4O      ; {@C514O2}            {MCM}
C514OOH         =  5C +  8H +  4O      ; {@C514OOH}           {MCM}
C59O2           =  5C +  9H +  5O      ; {@C59O2}             {MCM: HOCH2-CO-C(CH3)
(O2)-CH2OH}
C59OOH          =  5C + 10H +  5O      ; {@C59OOH}            {MCM: HOCH2-CO-C(CH3)
(OOH)-CH2OH}
C5H8            =  5C +  8H            ; {@C_5H_8}            {MCM:
CH2=C(CH3)CH=CH2 = isoprene}
CHOC3COCO3      =  5C +  5H +  5O      ; {@CHOC3COCO3}        {MCM}
CHOC3COOOH      =  5C +  6H +  4O      ; {@CHOC3COOOH}        {MCM}
CO13C4CHO       =  5C +  6H +  3O      ; {@CO13C4CHO}         {MCM}
CO23C4CHO       =  5C +  6H +  3O      ; {@CO23C4CHO}         {MCM}
CO23C4CO3       =  5C +  5H +  5O      ; {@CO23C4CO3}         {MCM}
CO23C4CO3H      =  5C +  6H +  5O      ; {@CO23C4CO3H}        {MCM}
DB1O            =  5C +  9H +  3O      ; {@DB1O2}             {Alkoxy radical which
undergoes the double H-shift predicted by T. Dibble and confirmed by F. Paulot}
DB1O2           =  5C +  9H +  4O      ; {@DB1O2}             {Peroxy radical with
a vinyl alcohol part}
DB1OOH          =  5C + 10H +  4O      ; {@DB1OOH}            {}
DB2O2           =  5C +  9H +  5O      ; {@DB1O2}             {}
DB2OOH          =  5C + 10H +  5O      ; {@DB2OOH}            {}
HCOC5           =  5C +  8H +  2O      ; {@HCOC5}             {MCM: HOCH2-CO-
C(CH3)=CH2}
ISOPAOH         =  5C + 10H +  2O      ; {@ISOPAOH}           {MCM: HOCH2-
C(CH3)=CH-CH2OH}
ISOPBO2         =  5C +  9H +  3O      ; {@ISOPBO2}           {MCM: HOCH2-C(CH3)
(O2)-CH=CH2}
ISOPBOH         =  5C + 10H +  2O      ; {@ISOPBOH}           {MCM: HOCH2-C(CH3)
(OH)-CH=CH2}
ISOPBOOH        =  5C + 10H +  3O      ; {@ISOPBOOH}          {MCM: HOCH2-C(CH3)
(OOH)-CH=CH2}
ISOPDO2         =  5C +  9H +  3O      ; {@ISOPDO2}           {MCM:
CH2=C(CH3)CH(O2)-CH2OH}
ISOPDOH         =  5C + 10H +  2O      ; {@ISOPDOH}           {MCM:
CH2=C(CH3)CH(OH)-CH2OH}
ISOPDOOH        =  5C + 10H +  3O      ; {@ISOPDOOH}          {MCM:
CH2=C(CH3)CH(OOH)-CH2OH}
MBO             =  5C + 10H +   O      ; {@MBO}               {MCM: 2-methyl-3-
buten-2-ol}
MBOACO          =  5C + 10H +  3O      ; {@MBOACO}            {MCM}
MBOCOCO         =  5C +  8H +  3O      ; {@MBOCOCO}           {MCM}
ME3FURAN        =  5C +  6H +   O      ; {@3METHYLFURAN}      {3-methyl-furan}
{5C aromatics (CHO)}
ACCOMECHO       =  5C +  6H +  4O      ; {@ACCOMECHO}         {MCM}
ACCOMECO3       =  5C +  5H +  6O      ; {@ACCOMECO3}         {MCM}
ACCOMECO3H      =  5C +  6H +  6O      ; {@ACCOMECO3H}        {MCM}
C24O3CCO2H      =  5C +  6H +  5O      ; {@C24O3CCO2H}        {MCM}
C4CO2DBCO3      =  5C +  3H +  5O      ; {@C4CO2DBCO3}        {MCM}
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C4CO2DCO3H      =  5C +  4H +  5O      ; {@C4CO2DCO3H}        {MCM}
C5134CO2OH      =  5C +  6H +  4O      ; {@C5134CO2OH}        {MCM: 2-hydroxy-3,4-
dioxopentanal}
C54CO           =  5C +  4H +  4O      ; {@C54CO}             {MCM: 2,3,4-
trioxopentanal}
C5CO14O2        =  5C +  5H +  4O      ; {@C5CO14O2}          {MCM}
C5CO14OH        =  5C +  6H +  3O      ; {@C5CO14OH}          {MCM: 4-oxo-2-
pentenoic acid}
C5CO14OOH       =  5C +  6H +  4O      ; {@C5CO14OOH}         {MCM}
C5DIALCO        =  5C +  4H +  3O      ; {@C5DIALCO}          {MCM}
C5DIALO2        =  5C +  5H +  4O      ; {@C5DIALO2}          {MCM}
C5DIALOOH       =  5C +  6H +  4O      ; {@C5DIALOOH}         {MCM}
C5DICARB        =  5C +  6H +  2O      ; {@C5DICARB}          {MCM: 4-oxo-2-
pentenal}
C5DICARBO2      =  5C +  7H +  5O      ; {@C5DICARBO2}        {MCM:
carboxy(hydroxy)acetate}
C5DICAROOH      =  5C +  8H +  5O      ; {@C5DICAROOH}        {MCM}
MC3ODBCO2H      =  5C +  6H +  3O      ; {@MC3ODBCO2H}        {MCM}
MMALANHY        =  5C +  4H +  3O      ; {@MMALANHY}          {MCM: 3-methyl-2,5-
furandione}
MMALANHYO2      =  5C +  5H +  6O      ; {@MMALANHYO2}        {MCM}
MMALNHYOOH      =  5C +  6H +  6O      ; {@MMALNHYOOH}        {MCM}
TLFUO2          =  5C +  7H +  5O      ; {@TLFUO2}            {MCM}
TLFUONE         =  5C +  6H +  2O      ; {@TLFUONE}           {MCM: 5-methyl-2(5H)-
furanone}
TLFUOOH         =  5C +  8H +  5O      ; {@TLFUOOH}           {MCM}
{5C (CHON)}
C4MCONO3OH      =  5C +  9H +  5O +  N ; {@C4MCONO3OH}        {MCM}
C514NO3         =  5C +  7H +  5O +  N ; {@C514NO3}           {MCM}
C5PAN9          =  5C +  5H +  7O +  N ; {@C5PAN9}            {MCM}
CHOC3COPAN      =  5C +  5H +  5O +  N ; {@CHOC3COPAN}        {MCM}
DB1NO3          =  5C +  9H +  6O +  N ; {@DB1NO3}            {}
ISOPBDNO3O2     =  5C + 10H +  7O +  N ; {@ISOPBDNO3O2}       {}
ISOPBNO3        =  5C +  9H +  4O +  N ; {@ISOPBNO3}          {MCM: HOCH2-C(CH3)
(ONO2)-CH=CH2}
ISOPDNO3        =  5C +  9H +  4O +  N ; {@ISOPDNO3}          {MCM:
CH2=C(CH3)CH(ONO2)-CH2OH}
NC4CHO          =  5C +  7H +  4O +  N ; {@NC4CHO}            {MCM: O2NOCH2-
C(CH3)=CH-CHO}
NC4OHCO3        =  5C +  8H +  6O +  N ; {@NC4OHCO3}          {MCM}
NC4OHCO3H       =  5C +  9H +  6O +  N ; {@NC4OHCO3H}         {MCM}
NC4OHCPAN       =  5C +  8H +  8O + 2N ; {@NC4OHCPAN}         {MCM}
NISOPO2         =  5C +  8H +  5O +  N ; {@NISOPO2}           {MCM: O2NOCH2-
C(CH3)=CH-CH2O2}
NISOPOOH        =  5C +  9H +  5O +  N ; {@NISOPOOH}          {MCM: O2NOCH2-
C(CH3)=CH-CH2OOH}
NMBOBCO         =  5C +  9H +  5O +  N ; {@NMBOBCO}           {MCM}
{5C aromatics (CHON)}
ACCOMEPAN       =  5C +  5H +  6O +  N ; {@ACCOMEPAN}         {MCM}
C4CO2DBPAN      =  5C +  3H +  7O +  N ; {@C4CO2DBPAN}        {MCM}
C5COO2NO2       =  5C +  5H +  6O +  N ; {@C5COO2NO2}         {MCM}
NC4MDCO2H       =  5C +  5H +  5O +  N ; {@NC4MDCO2H N}       {MCM}
NTLFUO2         =  5C +  6H +  7O +  N ; {@NTLFUO2}           {MCM}
NTLFUOOH        =  5C +  7H +  6O +  N ; {@NTLFUOOH}          {MCM}
{5C (CHO) (lumped)}
LC578O2         =  5C +  9H +  5O      ; {@LC578O2}           {HOCH2-CH(OH)C(CH3)
(O2)-CHO + HOCH2-C(CH3)(O2)-CH(OH)-CHO}
LC578OOH        =  5C + 10H +  5O      ; {@LC578OOH}          {HOCH2-CH(OH)C(CH3)
(OOH)-CHO + HOCH2-C(CH3)(OOH)-CH(OH)-CHO}
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LDISOPACO       =  5C +  9H +  2O      ; {@LISOPACO}          {}
LDISOPACO2      =  5C +  9H +  3O      ; {@LDISOPACO2}        {}
LHC4ACCHO       =  5C +  8H +  2O      ; {@LHC4ACCHO}         {HOCH2-C(CH3)=CH-CHO
+ HOCH2-CH=C(CH3)-CHO}
LHC4ACCO2H      =  5C +  8H +  3O      ; {@LHC4ACCO2H}        {HOCH2-C(CH3)=CH-
C(O)OH + HOCH2-CH=C(CH3)-C(O)OH}
LHC4ACCO3       =  5C +  7H +  4O      ; {@LHC4ACCO3}         {HOCH2-C(CH3)=CH-
C(O)O2 + HOCH2-CH=C(CH3)-C(O)O2}
LHC4ACCO3H      =  5C +  8H +  4O      ; {@LHC4ACCO3H}        {HOCH2-C(CH3)=CH-
C(O)OOH + HOCH2-CH=C(CH3)-C(O)OOH}
LIEPOX          =  5C + 10H +  3O      ; {@LIEPOX}            {epoxydiol}
LISOPAB         =  5C +  9H +   O      ; {@LISOPAB}           {}
LISOPACO        =  5C +  9H +  2O      ; {@LISOPACO}          {HOCH2-C(CH3)=CH-CH2O
+ HOCH2-CH=C(CH3)-CH2O}
LISOPACO2       =  5C +  9H +  3O      ; {@LISOPACO2}         {HOCH2-C(CH3)=CH-
CH2O2 + HOCH2-CH=C(CH3)-CH2O2}
LISOPACOOH      =  5C + 10H +  3O      ; {@LISOPACOOH}        {HOCH2-C(CH3)=CH-
CH2OOH + HOCH2-CH=C(CH3)-CH2OOH}
LISOPCD         =  5C +  9H +   O      ; {@LISOPCD}           {}
LISOPEFO        =  5C +  9H +  2O      ; {@LISOPEFO}          {}
LISOPEFO2       =  5C +  9H +  3O      ; {@LISOPEFO2}         {}
LMBOABO2        =  5C + 11H +  4O      ; {@LMBOABO2}          {}
LMBOABOOH       =  5C + 12H +  4O      ; {@LMBOABOOH}         {}
LME3FURANO2     =  5C +  7H +  4O      ; {@L3METHYLFURANO2}   {hydroxy-3-methyl-
furan peroxy radical}
LZCO3C23DBCOD   =  5C +  5H +  4O      ; {@LZCO3C23DBCOD}     {}
LZCO3HC23DBCOD  =  5C +  6H +  4O      ; {@LZCO3HC23DBCOD}    {C5PACALD1 +
C5PACALD2}
LZCODC23DBCOOH  =  5C +  8H +  3O      ; {@LZCODC23DBCOOH}    {C5HPALD1 + C5HPALD2}
{5C (CHON) (lumped)}
LC5PAN1719      =  5C +  7H +  6O +  N ; {@LC5PAN1719}        {HOCH2-C(CH3)=CH-
C(O)OONO2 + HOCH2-CH=C(CH3)C(O)OONO2}
LISOPACNO3      =  5C +  9H +  4O +  N ; {@LISOPACNO3}        {HOCH2-C(CH3)=CH-
CH2ONO2 + HOCH2-CH=C(CH3)-CH2ONO2}
LISOPACNO3O2    =  5C + 10H +  7O +  N ; {@LISOPACNO3O2}      {RO2 resulting from
OH-addition to ISOPANO3 and ISOPCNO3}
LMBOABNO3       =  5C + 11H +  5O +  N ; {@LMBOABNO3}         {}
LNISO3          =  5C              +  N ; {@LNISO3}           {C510O2+NC4CO3 = CHO-
CH(OH)-C(CH3)(O2)-CH2ONO2 + O2NOCH2-C(CH3)=CH-C(O)O2}
LNISOOH         =  5C              +  N ; {@LNISOOH}          {CHO-CH(OH)-C(CH3)
(OOH)-CH2ONO2 + O2NOCH2-C(CH3)=CH-C(O)OOH}
LNMBOABO2       =  5C +  9H +  6O +  N ; {@LNMBOABO2}         {}
LNMBOABOOH      =  5C + 10H +  6O +  N ; {@LNMBOABOOH}        {}
LZCPANC23DBCOD  =  5C +  5H +  6O +  N ; {@LZCPANC23DBCOD}    {}
{6C (CHO)}
C614CO          =  6C +  8H +  4O      ; {@C614CO}            {MCM}
C614O2          =  6C +  9H +  5O      ; {@C614O2}            {MCM}
C614OOH         =  6C + 10H +  5O      ; {@C614OOH}           {MCM}
CO235C5CHO      =  6C +  6H +  4O      ; {@CO235C5CHO}        {MCM}
CO235C6O2       =  6C +  7H +  5O      ; {@CO235C6O2}         {MCM}
CO235C6OOH      =  6C +  8H +  5O      ; {@CO235C6OOH}        {MCM}
{C6 (CHO) aromatics}
BENZENE         =  6C +  6H            ; {@BENZENE}           {MCM}
BZBIPERO2       =  6C +  7H +  5O      ; {@BZBIPERO2}         {MCM}
BZBIPEROOH      =  6C +  8H +  5O      ; {@BZBIPEROOH}        {MCM}
BZEMUCCO        =  6C +  6H +  5O      ; {@BZEMUCCO}          {MCM}
BZEMUCCO2H      =  6C +  6H +  4O      ; {@BZEMUCCO2H}        {MCM}
BZEMUCCO3       =  6C +  5H +  5O      ; {@BZEMUCCO3}         {MCM}
BZEMUCCO3H      =  6C +  6H +  5O      ; {@BZEMUCCO3H}        {MCM}
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BZEMUCO2        =  6C +  7H +  6O      ; {@BZEMUCO2}          {MCM}
BZEMUCOOH       =  6C +  8H +  6O      ; {@BZEMUCOOH}         {MCM}
BZEPOXMUC       =  6C +  6H +  3O      ; {@BZEPOXMUC}         {MCM}
BZOBIPEROH      =  6C +  6H +  4O      ; {@BZOBIPEROH}        {MCM}
C5CO2DBCO3      =  6C +  5H +  5O      ; {@C5CO2DBCO3}        {MCM}
C5CO2DCO3H      =  6C +  6H +  5O      ; {@C5CO2DCO3H}        {MCM}
C5CO2OHCO3      =  6C +  5H +  6O      ; {@C5CO2OHCO3}        {MCM}
C5COOHCO3H      =  6C +  6H +  6O      ; {@C5COOHCO3H}        {MCM}
C6125CO         =  6C +  6H +  3O      ; {@C6125CO}           {MCM: 2,5-dioxo-3-
hexenal}
C615CO2O2       =  6C +  7H +  4O      ; {@C615CO2O2}         {MCM}
C615CO2OOH      =  6C +  8H +  4O      ; {@C615CO2OOH}        {MCM}
C6CO4DB         =  6C +  4H +  4O      ; {@C6CO4DB}           {MCM}
C6H5O           =  6C +  5H +   O      ; {@C6H5O}             {MCM: phenyloxidanyl}
C6H5O2          =  6C +  5H +  2O      ; {@C6H5O2}            {MCM}
C6H5OOH         =  6C +  6H +  2O      ; {@C6H5OOH}           {MCM: phenyl
hydroperoxide}
CATEC1O         =  6C +  5H +  2O      ; {@CATEC1O}           {MCM: 2-λ1-
oxidanylphenol}
CATEC1O2        =  6C +  5H +  3O      ; {@CATEC1O2}          {MCM}
CATEC1OOH       =  6C +  6H +  3O      ; {@CATEC1OOH}         {MCM}
CATECHOL        =  6C +  4H +  2O      ; {@CATECHOL}          {MCM: catechol}
CPDKETENE       =  6C +  4H +   O      ; {@CPDKETENE}         {hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}
PBZQCO          =  6C +  4H +  4O      ; {@PBZQCO}            {MCM}
PBZQO2          =  6C +  5H +  5O      ; {@PBZQO2}            {MCM}
PBZQONE         =  6C +  4H +  2O      ; {@PBZQONE}           {MCM: 1,4-
benzoquinone}
PBZQOOH         =  6C +  6H +  5O      ; {@PBZQOOH}           {MCM}
PHENO2          =  6C +  7H +  6O      ; {@PHENO2}            {MCM}
PHENOL          =  6C +  6H +   O      ; {@PHENOL}            {MCM}
PHENOOH         =  6C +  8H +  6O      ; {@PHENOOH}           {MCM}
{6C (CHON)}
C614NO3         =  6C +  9H +  6O +  N ; {@C614NO3}           {MCM}
{C6 (CHON) aromatics}
BZBIPERNO3      =  6C +  7H +  6O +  N ; {@BZBIPERNO3}        {MCM}
BZEMUCNO3       =  6C +  7H +  7O +  N ; {@BZEMUCNO3}         {MCM}
BZEMUCPAN       =  6C +  5H +  7O +  N ; {@BZEMUCPAN}         {MCM}
C5CO2DBPAN      =  6C +  5H +  7O +  N ; {@C5CO2DBPAN}        {MCM}
C5CO2OHPAN      =  6C +  5H +  8O +  N ; {@C5CO2OHPAN}        {MCM}
DNPHEN          =  6C +  4H +  5O + 2N ; {@DNPHEN}            {MCM: 2,4-
dinitrophenol}
DNPHENO2        =  6C +  5H + 10O + 2N ; {@DNPHENO2}          {MCM}
DNPHENOOH       =  6C +  6H + 10O + 2N ; {@DNPHENOOH}         {MCM}
HOC6H4NO2       =  6C +  5H +  3O +  N ; {@HOC6H4NO2}         {MCM: 2-nitrophenol}
NBZQO2          =  6C +  4H +  7O +  N ; {@NBZQO2}            {MCM}
NBZQOOH         =  6C +  5H +  7O +  N ; {@NBZQOOH}           {MCM}
NCATECHOL       =  6C +  5H +  4O +  N ; {@NCATECHOL}         {MCM}
NCATECO2        =  6C +  6H +  9O +  N ; {@NCATECO2}          {MCM}
NCATECOOH       =  6C +  7H +  9O +  N ; {@NCATECOOH}         {MCM}
NCPDKETENE      =  6C +  3H +  3O +  N ; {@NCPDKETENE}        {hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}
NDNPHENO2       =  6C +  4H + 12O + 3N ; {@NDNPHENO2}         {MCM}
NDNPHENOOH      =  6C +  5H + 12O + 3N ; {@NDNPHENOOH}        {MCM}
NNCATECO2       =  6C +  5H + 11O + 2N ; {@NNCATECO2}         {MCM}
NNCATECOOH      =  6C +  6H + 11O + 2N ; {@NNCATECOOH}        {MCM}
NPHEN1O         =  6C +  4H +  3O +  N ; {@NPHEN1O}           {MCM}
NPHEN1O2        =  6C +  4H +  4O +  N ; {@NPHEN1O2}          {MCM}
NPHEN1OOH       =  6C +  5H +  4O +  N ; {@NPHEN1OOH}         {MCM}
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NPHENO2         =  6C +  6H +  8O +  N ; {@NPHENO2}          {MCM}
NPHENOOH        =  6C +  7H +  8O +  N ; {@NPHENOOH}         {MCM}
{7C (CHO)}
C235C6CO3H      =  7C +  8H +  6O      ; {@C235C6CO3H}       {MCM}
C716O2          =  7C +  9H +  5O      ; {@C716O2}           {MCM}
C716OOH         =  7C + 10H +  5O      ; {@C716OOH}          {MCM}
C721O2          =  7C + 11H +  4O      ; {@C721O2}           {MCM}
C721OOH         =  7C + 12H +  4O      ; {@C721OOH}          {MCM}
C722O2          =  7C + 11H +  5O      ; {@C722O2}           {MCM}
C722OOH         =  7C + 12H +  5O      ; {@C722OOH}          {MCM}
CO235C6CHO      =  7C +  8H +  4O      ; {@CO235C6CHO}       {MCM}
CO235C6CO3      =  7C +  7H +  6O      ; {@CO235C6CO3}       {MCM}
MCPDKETENE      =  7C +  6H +  2O      ; {@MCPDKETENE}       {hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}
ROO6R3O         =  7C + 11H +  4O      ; {@ROO6R3O}          {from ref3019}
ROO6R3O2        =  7C + 11H +  5O      ; {@ROO6R3O2}         {ROO6R3OO from
ref3019}
ROO6R5O2        =  7C + 11H +  7O      ; {@ROO6R5O2}         {ROO6R5OO from
ref3019}
{C7 (CHO) aromatics}
BENZAL          =  7C +  6H +   O      ; {@BENZAL}           {MCM}
C6CO2OHCO3      =  7C +  7H +  6O      ; {@C6CO2OHCO3}       {MCM}
C6COOHCO3H      =  7C +  8H +  6O      ; {@C6COOHCO3H}       {MCM}
C6H5CH2O2       =  7C +  7H +  2O      ; {@C6H5CH2O2}        {MCM:
benzyldioxidanyl}
C6H5CH2OOH      =  7C +  8H +  2O      ; {@C6H5CH2OOH}       {MCM: benzyl
hydroperoxide}
C6H5CO3         =  7C +  5H +  3O      ; {@C6H5CO3}          {MCM}
C6H5CO3H        =  7C +  6H +  3O      ; {@C6H5CO3H}         {MCM: perbenzoic
acid}
C7CO4DB         =  7C +  6H +  4O      ; {@C7CO4DB}          {MCM}
CRESO2          =  7C +  9H +  6O      ; {@CRESO2}           {MCM}
CRESOL          =  7C +  8H +   O      ; {@CRESOL}           {MCM: 2-methylphenol}
CRESOOH         =  7C + 10H +  6O      ; {@CRESOOH}          {MCM}
MCATEC1O        =  7C +  7H +  2O      ; {@MCATEC1O}         {MCM}
MCATEC1O2       =  7C +  7H +  3O      ; {@MCATEC1O2}        {MCM}
MCATEC1OOH      =  7C +  8H +  3O      ; {@MCATEC1OOH}       {MCM}
MCATECHOL       =  7C +  8H +  2O      ; {@MCATECHOL}        {MCM: 3-
methylcatechol}
OXYL1O2         =  7C +  7H +  2O      ; {@OXYL1O2}          {MCM: 1-methyl-2-
(oxo-λ3-oxidanyl)benzene}
OXYL1OOH        =  7C +  8H +  2O      ; {@OXYL1OOH}         {MCM}
PHCOOH          =  7C +  6H +  2O      ; {@PHCOOH}           {MCM: benzoic acid}
PTLQCO          =  7C +  6H +  4O      ; {@PTLQCO}           {MCM}
PTLQO2          =  7C +  7H +  5O      ; {@PTLQO2}           {MCM}
PTLQONE         =  7C +  6H +  2O      ; {@PTLQONE}          {MCM: 2-methyl-1,4-
benzoquinone}
PTLQOOH         =  7C +  8H +  5O      ; {@PTLQOOH}          {MCM}
TLBIPERO2       =  7C +  9H +  5O      ; {@TLBIPERO2}        {MCM}
TLBIPEROOH      =  7C + 10H +  5O      ; {@TLBIPEROOH}       {MCM}
TLEMUCCO        =  7C +  8H +  5O      ; {@TLEMUCCO}         {MCM}
TLEMUCCO2H      =  7C +  8H +  4O      ; {@TLEMUCCO2H}       {MCM}
TLEMUCCO3       =  7C +  7H +  5O      ; {@TLEMUCCO3}        {MCM}
TLEMUCCO3H      =  7C +  8H +  5O      ; {@TLEMUCCO3H}       {MCM}
TLEMUCO2        =  7C +  9H +  6O      ; {@TLEMUCO2}         {MCM}
TLEMUCOOH       =  7C + 10H +  6O      ; {@TLEMUCOOH}        {MCM}
TLEPOXMUC       =  7C +  8H +  3O      ; {@TLEPOXMUC}        {MCM}
TLOBIPEROH      =  7C +  8H +  4O      ; {@TLOBIPEROH}       {MCM}
TOL1O           =  7C +  7H +   O      ; {@TOL1O}            {MCM: (2-
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methylphenyl)oxidanyl}
TOLUENE         =  7C +  8H            ; {@TOLUENE}          {MCM}
{7C (CHON)}
C7PAN3          =  7C +  7H +  8O +  N ; {@C7PAN3}           {MCM}
{C7 (CHON) aromatics}
C6CO2OHPAN      =  7C +  7H +  8O +  N ; {@C6CO2OHPAN}       {MCM}
C6H5CH2NO3      =  7C +  7H +  3O +  N ; {@C6H5CH2NO3}       {MCM: benzyl nitrate}
DNCRES          =  7C +  6H +  5O + 2N ; {@DNCRES}           {MCM: 2-methyl-4,6-
dinitrophenol}
DNCRESO2        =  7C +  7H + 10O + 2N ; {@DNCRESO2}         {MCM}
DNCRESOOH       =  7C +  8H + 10O + 2N ; {@DNCRESOOH}        {MCM}
MNCATECH        =  7C +  7H +  4O +  N ; {@MNCATECH}         {MCM: 3-methyl-6-
nitro-1,2-benzenediol}
MNCATECO2       =  7C +  8H +  9O +  N ; {@MNCATECO2}        {MCM}
MNCATECOOH      =  7C +  9H +  9O +  N ; {@MNCATECOOH}       {MCM}
MNCPDKETENE     =  7C +  5H +  3O +  N ; {@MNCPDKETENE}      {hv nitrophenol:
cyclopentadiene ketene (Luc Vereecken's prediction)}
MNNCATCOOH      =  7C +  8H + 11O + 2N ; {@MNNCATCOOH}       {MCM}
MNNCATECO2      =  7C +  7H + 11O + 2N ; {@MNNCATECO2}       {MCM}
NCRES1O         =  7C +  6H +  3O +  N ; {@NCRES1O}          {MCM}
NCRES1O2        =  7C +  6H +  4O +  N ; {@NCRES1O2}         {MCM}
NCRES1OOH       =  7C +  7H +  4O +  N ; {@NCRES1OOH}        {MCM}
NCRESO2         =  7C +  8H +  8O +  N ; {@NCRESO2}          {MCM}
NCRESOOH        =  7C +  9H +  8O +  N ; {@NCRESOOH}         {MCM}
NDNCRESO2       =  7C +  6H +  2O + 3N ; {@NDNCRESO2}        {MCM}
NDNCRESOOH      =  7C +  7H + 12O + 3N ; {@NDNCRESOOH}       {MCM}
NPTLQO2         =  7C +  6H +  7O +  N ; {@NPTLQO2}          {MCM}
NPTLQOOH        =  7C +  7H +  7O +  N ; {@NPTLQOOH}         {MCM}
PBZN            =  7C +  5H +  5O +  N ; {@PBZN}             {MCM: benzoyl nitro
peroxide}
TLBIPERNO3      =  7C +  9H +  6O +  N ; {@TLBIPERNO3}       {MCM}
TLEMUCNO3       =  7C +  9H +  7O +  N ; {@TLEMUCNO3}        {MCM}
TLEMUCPAN       =  7C +  7H +  7O +  N ; {@TLEMUCPAN}        {MCM}
TOL1OHNO2       =  7C +  7H +  3O +  N ; {@TOL1OHNO2}        {MCM: 2-methyl-6-
nitrophenol}
{8C (CHO)}
C721CHO         =  8C + 12H +  3O      ; {@C721CHO}          {MCM}
C721CO3         =  8C + 11H +  5O      ; {@C721CO3}          {MCM}
C721CO3H        =  8C + 12H +  5O      ; {@C721CO3H}         {MCM}
C810O2          =  8C + 13H +  4O      ; {@C810O2}           {MCM}
C810OOH         =  8C + 14H +  4O      ; {@C810OOH}          {MCM}
C811O2          =  8C + 13H +  4O      ; {@C811O2}           {MCM}
C812O2          =  8C + 13H +  5O      ; {@C812O2}           {MCM}
C812OOH         =  8C + 14H +  5O      ; {@C812OOH}          {MCM}
C813O2          =  8C + 13H +  6O      ; {@C813O2}           {MCM}
C813OOH         =  8C + 14H +  5O      ; {@C813OOH}          {MCM}
C85O2           =  8C + 13H +  3O      ; {@C85O2}            {MCM}
C85OOH          =  8C + 14H +  3O      ; {@C85OOH}           {MCM}
C86O2           =  8C + 13H +  4O      ; {@C86O2}            {MCM}
C86OOH          =  8C + 14H +  4O      ; {@C86OOH}           {MCM}
C89O2           =  8C + 13H +  3O      ; {@C89O2}            {MCM}
C89OOH          =  8C + 14H +  3O      ; {@C89OOH}           {MCM}
C8BC            =  8C + 14H            ; {@C8BC}             {MCM}
C8BCCO          =  8C + 12H +  O       ; {@C8BCCO}           {MCM}
C8BCO2          =  8C + 11H +  2O      ; {@C8BCO2}           {MCM}
C8BCOOH         =  8C + 12H +  2O      ; {@C8BCOOH}          {MCM}
NORPINIC        =  8C + 12H +  4O      ; {@NORPINIC}         {MCM}
{C8 (CHO) aromatics}
EBENZ           =  8C + 10H            ; {@EBENZ}            {MCM: ethylbenzene}
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STYRENE         =  8C +  8H            ; {@STYRENE}           {MCM}
STYRENO2        =  8C +  9H +  3O      ; {@STYRENO2}          {MCM}
STYRENOOH       =  8C + 10H +  3O      ; {@STYRENOOH}         {MCM}
{8C (CHON)}
C721PAN         =  8C + 11H +  7O +  N ; {@C721PAN}           {MCM}
C810NO3         =  8C + 14H +  5O +  N ; {@C810NO3}           {MCM}
C89NO3          =  8C + 13H +  4O +  N ; {@C89NO3}            {MCM}
C8BCNO3         =  8C + 11H +  3O +  N ; {@C8BCNO3}           {MCM}
{C8 (CHON) aromatics}
NSTYRENO2       =  8C +  8H +  5O +  N ; {@NSTYRENO2}         {MCM}
NSTYRENOOH      =  8C +  9H +  5O +  N ; {@NSTYRENOOH}        {MCM}
{C8 aromatics (lumped)}
LXYL            =  8C + 10H            ; {@LXYL}              {xylenes}
{9C (CHO)}
C811CO3         =  9C + 13H +  5O      ; {@C811CO3}           {MCM}
C811CO3H        =  9C + 14H +  5O      ; {@C811CO3H}          {MCM}
C85CO3          =  9C + 11H +  4O      ; {@C85CO3}            {MCM}
C85CO3H         =  9C + 12H +  4O      ; {@C85CO3H}           {MCM}
C89CO2H         =  9C + 14H +  3O      ; {@C89CO2H}           {MCM}
C89CO3          =  9C + 13H +  4O      ; {@C89CO3}            {MCM}
C89CO3H         =  9C + 14H +  4O      ; {@C89CO3H}           {MCM}
C96O2           =  9C + 15H +  3O      ; {@C96O2}             {MCM}
C96OOH          =  9C + 16H +  3O      ; {@C96OOH}            {MCM}
C97O2           =  9C + 15H +  4O      ; {@C97O2}             {MCM}
C97OOH          =  9C + 16H +  4O      ; {@C97OOH}            {MCM}
C98O2           =  9C + 15H +  5O      ; {@C98O2}             {MCM}
C98OOH          =  9C + 16H +  5O      ; {@C98OOH}            {MCM}
NOPINDCO        =  9C + 12H +  2O      ; {@NOPINDCO}          {MCM}
NOPINDO2        =  9C + 13H +  3O      ; {@NOPINDO2}          {MCM}
NOPINDOOH       =  9C + 14H +  3O      ; {@NOPINDOOH}         {MCM}
NOPINONE        =  9C + 14H +   O      ; {@NOPINONE}          {MCM}
NOPINOO         =  9C + 14H +  2O      ; {@NOPINOO}           {MCM}
NORPINAL        =  9C + 14H +  2O      ; {@NORPINAL}          {MCM: norpinaldehyde}
NORPINENOL      =  9C + 14H +  2O      ; {@NORPINENOL}        {}
PINIC           =  9C + 14H +  4O      ; {@PINIC}             {MCM: pinic acid}
{9C (CHON)}
C811PAN         =  9C + 13H +  7O +  N ; {@C811PAN}           {MCM}
C89PAN          =  9C + 13H +  5O +  N ; {@C89PAN}            {MCM}
C96NO3          =  9C + 15H +  4O +  N ; {@C96NO3}            {MCM}
C9PAN2          =  9C + 13H +  6O +  N ; {@C9PAN2}            {MCM}
{C9 aromatics (lumped)}
LTMB            =  9C + 12H            ; {@LTMB}              {trimethylbenzenes}
{10C (CHO)}
APINAOO         = 10C + 16H +  3O      ; {@APINAOO}           {stabilized APINOOA}
APINBOO         = 10C + 16H +  3O      ; {@APINBOO}           {MCM}
APINENE         = 10C + 16H            ; {@APINENE}           {MCM: alpha pinene}
BPINAO2         = 10C + 17H +  3O      ; {@BPINAO2}           {MCM}
BPINAOOH        = 10C + 18H +  3O      ; {@BPINAOOH}          {MCM}
BPINENE         = 10C + 16H            ; {@BPINENE}           {MCM: beta pinene}
C106O2          = 10C + 15H +  5O      ; {@C106O2}            {MCM}
C106OOH         = 10C + 16H +  5O      ; {@C106OOH}           {MCM}
C109CO          = 10C + 10H +  3O      ; {@C109CO}            {MCM}
C109O2          = 10C + 15H +  4O      ; {@C109O2}            {MCM}
C109OOH         = 10C + 16H +  4O      ; {@C109OOH}           {MCM}
C96CO3          = 10C + 15H +  4O      ; {@C96CO3}            {MCM}
CAMPHENE        = 10C + 16H            ; {@CAMPHENE}          {}
CARENE          = 10C + 16H            ; {@CARENE}            {3-carene}
MENTHEN6ONE     = 10C + 16H +  3O      ; {@MENTHEN6ONE}       {8-OOH-menthen-6-one,
Taraborrelli, pers. comm.}
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OH2MENTHEN6ONE  = 10C + 17H +  4O      ; {@2OHMENTHEN6ONE}    {2-OH-8-OOH-menthen-
6-one, Taraborrelli, pers. comm.}
OHMENTHEN6ONEO2 = 10C + 17H +  5O      ; {@OHMENTHEN6ONEO2}   {2-OH-8-OOH_menthen-
6-peroxy radical, Taraborrelli, pers. comm.}
PERPINONIC      = 10C + 16H +  4O      ; {@PERPINONIC}        {MCM}
PINAL           = 10C + 16H +  2O      ; {@PINAL}             {MCM: pinonaldehyde}
PINALO2         = 10C + 13H +  4O      ; {@PINALO2}           {MCM}
PINALOOH        = 10C + 14H +  4O      ; {@PINALOOH}          {MCM}
PINENOL         = 10C + 16H +  2O      ; {@PINEOL}            {}
PINONIC         = 10C + 16H +  3O      ; {@PINONIC}           {MCM: pinonic acid}
RO6R1O2         = 10C + 17H +  4O      ; {@RO6R1O2}           {cyclo-oxy peroxy
radical from BPINENE, ref3019}
RO6R3O2         = 10C + 17H +  5O      ; {@RO6R3O2}           {cyclo-oxy peroxy
radical from BPINENE, ref3019}
ROO6R1O2        = 10C + 17H +  5O      ; {@ROO6R1O2}          {cyclo-peroxy peroxy
radical from BPINENE based on ROO6R1 from ref3019}
SABINENE        = 10C + 16H            ; {@SABINENE}          {}
{10C (CHON)}
BPINANO3        = 10C + 17H +  4O +  N ; {@BPINANO3}          {MCM}
C106NO3         = 10C + 15H +  6O +  N ; {@C106NO3}           {MCM}
C10PAN2         = 10C + 15H +  6O +  N ; {@C10PAN2}           {MCM}
PINALNO3        = 10C + 13H +  5O +  N ; {@PINALNO3}          {MCM}
RO6R1NO3        = 10C + 17H +  5O +  N ; {@RO6R1NO3}          {nitrate from cyclo-
oxy peroxy radical from BPINENE, ref3019}
ROO6R1NO3       = 10C + 17H +  6O +  N ; {@ROO6R1NO3}         {nitrate from cyclo-
peroxy peroxy radical from BPINENE, ref3019}
{10C (lumped)}
LAPINABNO3      = 10C + 17H +  4O +  N ; {@LAPINABNO3}        {APINANO3 + APINBNO3
lumped (ratio 1:2)}
LAPINABO2       = 10C + 17H +  3O      ; {@LAPINABO2}         {APINAO2 + APINBO2
lumped (ratio 1:2)}
LAPINABOOH      = 10C + 18H +  3O      ; {@LAPINABOOH}        {APINAOOH + APINBOOH
lumped (ratio 1:2)}
LNAPINABO2      = 10C + 16H +  5O +  N ; {@LNAPINABO2}        {.65 NAPINAO2 + .35
NAPINBO2}
LNAPINABOOH     = 10C + 17H +  5O +  N ; {@LNAPINABOOH}       {.65 NAPINAOOH + .35
NAPINBOOH}
LNBPINABO2      = 10C + 16H +  5O +  N ; {@LNBPINABO2}        {.8 NBPINAO2 + .2
NBPINBO2}
LNBPINABOOH     = 10C + 17H +  5O +  N ; {@LNBPINABOOH}       {.8 NBPINAO2 + .2
NBPINBO2}
{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}
CH3I            =  C + 3H                     +  I ; {@CH_3I}
{iodomethane}
HI              =       H                     +  I ; {@HI}                {hydrogen
iodide}
HIO3            =       H + 3O                +  I ; {@HIO_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}
INO2            =           2O + N            +  I ; {@INO_2}             {iodine
nitrite}
INO3            =           3O + N            +  I ; {@INO_3}             {iodine
nitrate}
IO              =            O                +  I ; {@IO}                {iodine
monoxide radical}
IPART           =                               2I ; {@I(part)}           {iodine
particles}
OIO             =           2O                +  I ; {@OIO}               {}

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

CH3SO2          =  C + 3H + 2O    + S ; {@CH_3SO_2}          {}
CH3SO3          =  C + 3H + 3O    + S ; {@CH_3SO_3}          {}
CH3SO3H         =  C + 4H + 3O    + S ; {@CH_3SO_3H}         {MSA: methane sulfonic
acid}
DMS             = 2C + 6H         + S ; {@DMS}               {dimethyl sulfide}
```

```
DMSO            = 2C + 6H +  O    + S ; {@DMSO}              {dimethyl sulfoxide:
CH3SOCH3}
H2SO4           =      2H + 4O    + S ; {@H_2SO_4}           {sulfuric acid}
OCS             =  C      +  O    + S ; {@OCS}               {}
S               =                  S ; {@S}                 {sulfur atomic ground
state}
SF6             =              6F + S ; {@SF_6}              {sulfur hexaflouride}
SH              =       H          + S ; {@SH}                {}
SO              =            O     + S ; {@SO}                {sulfur monoxide}
SO2             =           2O     + S ; {@SO_2}              {sulfur dioxide}
SO3             =           3O     + S ; {@SO_3}              {sulfur trioxide}
LSULFUR         =                  S ; {@LSULFUR}           {lumped S species}

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

Hg              = Hg                    ; {@Hg}                {}
HgO             = Hg + O                ; {@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 + O + 2Br          ; {@BrHgOBr}           {}
ClHgOBr         = Hg + O + Cl + Br      ; {@ClHgOBr}           {}

{--- mz_pj_20070209+}
{------------------------ Pseudo Aerosol ---------------------------------}
NO3m_cs         = N + 3O                ; {@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+}
{------------------------ O3 Budget Tracers (via eval2.3.rpl) -------------}
O3s             = 3O                    ; {@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 + 3O          ; {@ISO2}              {isoprene (hydroxy)
peroxy radicals}
ISON            = 5C +           N      ; {@ISON}              {organic nitrates
from ISO2 and C5H8+NO3}
ISOOH           = 5C + 10H + 3O         ; {@ISOOH}             {isoprene (hydro)
peroxides}
LHOC3H6O2       = 3C + 7H + 3O          ; {@CH_3CH(O_2)CH_2OH} {hydroxyperoxyradical
from propene+OH}
LHOC3H6OOH      = 3C + 8H + 3O          ; {@CH_3CH(OOH)CH_2OH} {C3H6OHOOH =
hydroxyhydroperoxides from C3H6}
MVKO2           = 4C + 7H + 4O          ; {@MVKO2}             {MVK/MACR peroxy
radicals}
```

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

{ mz_ab_20100908+}
{---------------------------------- ions -------------------------------------}
Op              =  O           + Pls    ; {@O^+}                {O+}
O2p             =  2O          + Pls    ; {@O_2^+}              {O2+}
Np              =  N           + Pls    ; {@N^+}                {N+}
N2p             =  2N          + Pls    ; {@N_2^+}              {N2+}
NOp             =  O + 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           = O + 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 Condesable Gases and VOCs--------------------}
LTERP           =  IGNORE               ; {@LTERP}              {terpenes}
LALK4           =  IGNORE               ; {@LALK4}              {alkanes}
LALK5           =  IGNORE               ; {@LALK5}              {alkanes}
LARO1           =  IGNORE               ; {@LARO1}              {aromatic VOC}
LARO2           =  IGNORE               ; {@LARO2}              {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}
{ mz_at_20131015- needed for ORACLE.rpl}

{ mz_rs_20170601+ jam}
ACBZO2          =                     5H + 7C + 3O ; {@C_7H_5O_3}             {acyl
peroxy radical from benzaldehyde}
ALKNO3          =               11H + 5C + 3O +  N ; {@C_5H_<11>NO_3}
{nitrate from BIGALKANE}
ALKO2           =                    11H + 5C + 2O ; {@C_5H_<11>O_2}
{peroxy radical from large alkanes}
ALKOH           =                    12H + 5C +  O ; {@C_5H_<12>O}
{alcohol from BIGALKANE}
ALKOOH          =                    12H + 5C + 2O ; {@C_5H_<12>O_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}
BENZO2          =                     7H + 6C + 5O ; {@C_6H_7O_5}
```

```
{peroxy radical from benzene}
BENZOOH         =                      8H + 6C + 5O ; {@C_6H_8O_5}
{peroxide from BENZO2}
BEPOMUC         =                      6H + 6C + 3O ; {@C_6H_6O_3}
{benzene eopoxy diol}
BIGALD1         =                      4H + 4C + 2O ; {@C_4H_4O_2}             {but-
2-enedial}
BIGALD2         =                      6H + 5C + 2O ; {@C_5H_6O_2}             {4-
oxopent-2-enal}
BIGALD3         =                      6H + 5C + 2O ; {@C_5H_6O_2}             {2-
methylbut-2-enedial}
BIGALD4         =                      8H + 6C + 2O ; {@C_6H_8O_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 +  O ; {@C_7H_6O}
{benzaldehyde}
BZOO            =                      7H + 7C + 2O ; {@C_7H_7O_2}
{peroxy radical from toluene}
BZOOH           =                      8H + 7C + 2O ; {@C_7H_8O_2}
{peroxide from BZOO}
C3H7O2          =                      7H + 3C + 2O ; {@C_3H_7O_2}
{lumped peroxy radical from propane}
C3H7OOH         =                      8H + 3C + 2O ; {@C_3H_8O_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 +  O + 2F ; {@CF_2O}
{carbonyl difluoride}
COFCL           =                C +  F +  O +  Cl ; {@CFClO}
{carbonyl chloride fluoride}
DICARBO2        =                      5H + 5C + 4O ; {@C_5H_5O_4}
{dicarbonyl from photolysis of BIGALD2}
ELVOC           = IGNORE                                ; {@ELVOC}
ENEO2           =                      9H + 4C + 3O ; {@C_4H_9O_3}
{peroxy radical from BIGENE/OLTP}
EOOH            =                      6H + 2C + 3O ; {@C_2H_6O_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-
chloro-1,1-difluoroethane}
HCFC22          =                 H +  C + 2F +  Cl ; {@CHF_2Cl}
{chloro(difluoro)methane}
HF              =                           H +  F ; {@HF}
{fluorane}
```

```
HOCH2OO         =                      3H +  C + 3O ; {@CH_3O_3}
{(hydroxymethyl)dioxidanyl}
HPALD           = IGNORE                            ; {@HPALD}
IEC1O2          =                      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}
LISOPNO3NO3     = IGNORE                            ; {@LISOPNO3NO3}
LISOPNO3O2      = IGNORE                            ; {@LISOPNO3O2}
LISOPNO3OOH     = IGNORE                            ; {@LISOPNO3OOH}
LISOPOOHO2      = IGNORE                            ; {@LISOPOOHO2}
LISOPOOHOOH     = IGNORE                            ; {@LISOPOOHOOH}
MALO2           =                      3H + 4C + 4O ; {@C_4H_3O_4}
{peroxy radical from photolysis of BIGALD1}
MBONO3O2        =                10H + 5C + 6O +  N ; {@C_5H_<10>NO_6}
{peroxy nitrate radical from MBO+NO3}
MBOO2           =                     11H + 5C + 4O ; {@C_5H_<11>O_4}
{peroxy radical from MBO}
MBOOOH          =                     12H + 5C + 4O ; {@C_5H_<12>O_4}
{peroxide from MBO}
MDIALO2         =                      5H + 5C + 4O ; {@C_5H_5O_4}
{peroxy radical from photolysis of BIGALD3}
MEKNO3          = IGNORE                            ; {@MEKNO3}
MVKN            = IGNORE                            ; {@MVKN}
MYRC            =                         16H + 10C ; {@C_<10>H_<16>}          {2-
methyl-6-methylideneocta-1,7-diene}
NTERPNO3        = IGNORE                            ; {@NTERPNO3}
NTERPO2         =              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}
TERP2O2         =                    15H + 10C + 4O ; {@C_<10>H_<15>O_4}
{peroxy radical from TERPROD1}
TERP2OOH        =                    16H + 10C + 4O ; {@C_<10>H_<16>O_4}
{peroxide from TERP2O2}
TERPNO3         =              17H + 10C + 4O +  N ; {@C_<10>H_<17>NO_4}
{nitrate from terpenes}
TERPO2          =                    17H + 10C + 3O ; {@C_<10>H_<17>O_3}
{peroxy radical from terpenes}
TERPOOH         =                    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}
TOLO2           =                      9H + 7C + 5O ; {@C_7H_9O_5}
{peroxy radical from toluene}
TOLOOH          =                     10H + 7C + 5O ; {@C_7H_<10>O_5}
{peroxide from toluene}
XYLENO2         =                     11H + 8C + 5O ; {@C_8H_<11>O_5}
```

```
{peroxy radical from xylene}
XYLENOOH        =                   12H + 8C + 5O ; {@C_8H_<12>O_5}
{peroxide from XYLENO2}
XYLOL           =                   10H + 8C +  O ; {@C_8H_<10>O}            {2,3-
dimethylphenol}
XYLOLO2         =                   11H + 8C + 6O ; {@C_8H_<11>O_6}
{peroxy radical from xylol}
XYLOLOOH        =                   12H + 8C + 6O ; {@C_8H_<12>O_6}
{peroxide from xylol}
{ mz_rs_20170601-}

{ mz_rs_20171213+ MOZART}
O2_1D           = 2O                ; {@O_2}              {excited molecular
oxygen (singlett D state)}
O2_1S           = 2O                ; {@O_2}              {excited molecular
oxygen (singlett S state)}
ONIT            =  3C +  5H + 4O + N ; {@C_3H_5NO_4}       {organic nitrate}
C4H8            =  4C +  8H          ; {@C4H8}             {large alkenes}
C4H9O3          =  4C +  9H + 3O     ; {@C_4H_9O_3}        {peroxy radical from
C4H8}
C5H12           =  5C + 12H          ; {@C5H12}            {large alkanes}
C5H11O2         =  5C + 11H + 2O     ; {@C5H11O2}          {peroxy radical from
large alkanes}
C5H6O2          =  5C +  6H + 2O     ; {@C5H6O2}           {aldehyde from toluene
oxidation}
HYDRALD         =  5C +  8H + 2O     ; {@C_5H_8O_2}        {lumped unsaturated
hydroxycarbonyl}
ISOPO2          =  5C +  9H + 3O     ; {@C_5H_9O_3}        {lumped peroxy radical
from isoprene}
C5H9O3          =  5C +  9H + 4O     ; {@C_5H_9O_4}        {peroxy radical from
OH+HYDRALD}
ISOPOOH         =  5C + 10H + 3O     ; {@C_5H_10O_3}       {peroxide from
isoprene}
C5H12O2         =  5C + 12H + 2O     ; {@C5H12O2}          {peroxide from large
alkanes}
ONITR           =  5C +  9H + 4O + N ; {@C_5H_9NO_4}       {alkyl nitrate from
ISOPO2+NO3}
C5H10O4         =  5C + 10H + 4O     ; {@C_5H_10O_4}       {peroxide from C5H9O3}
ROO6R5P         =  7C + 10H + 6O     ; {@ROO6R5P}          {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 +  O      ; {@HCO}              {CHO formyl radical}
ISPD            =  4C +  6H +  O     ; {@ISPD}             {lumped MACR MVK}
ClOO            = Cl + 2O            ; {@CLOO}             {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}
ACO2            = IGNORE             ; {@ACO2}             {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}
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          =      3O + 2N        ; {@N_2O_3}           {dinitrogen trioxide}
N2O4          =      4O + 2N        ; {@N_2O_4}           {dinitrogen
tetraoxide}

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

{1C (amines)}

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

{2C (amines)}

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

{3C (amines)}

TMA           = 3C + 9H      + N      ; {@TMA}               {trimethylamine}
TMAO2         = 3C + 8H + 2O + N      ; {@TMAO2}             {TMA-peroxyradical}
TMAO          = 3C + 8H + O  + N      ; {@TMAO}              {alkoxy-radical of
TMA}
DMNCHO        = 3C + 7H + O  + N      ; {@DMNCHO}            {N,N-dimethyl
formamide}
DMNCHOO2      = 3C + 6H + 3O + N      ; {@DMNCHOO2}          {peroxyradical of N,N-
dimethyl formamide}
TMADF         = 3C + 5H + 2O + N      ; {@TMADF}             {N-methyl diformamide}
HOETNHCHO     = 3C + 7H + 2O + N      ; {@HOETNHCHO}         {ethanol amide}
HOCH2CONHCHO  = 3C + 5H + 3O + N      ; {@HOCH2CONHCHO}      {hydroxyaceto
formamide}
DMCNH2        = 3C + 8H + N           ; {@DMCNH2}            {amino propyl radical}
DMCOONH2      = 3C + 8H + 2O + N      ; {@DMCOONH2}          {amino propyl
peroxyradical}
CH2CNH2CH3    = 3C + 7H + N           ; {@CH2CNH2CH3}        {2-amino propene}
DMCNH         = 3C + 7H + N           ; {@DMCNH}             {2-propane imine}
CH3CNH2MOH    = 3C + 8H + O  + N      ; {@CH3CNH2MOH}        {amino propanol
radical}
H2NCCHOHCH3   = 3C + 7H + O  + N      ; {@H2NCCHOHCH3}       {2-aminoprop-2-en-1-
ol}
HNCCH3MOH     = 3C + 7H + O  + N      ; {@HNCCH3MOH}         {2-iminopropan-1-ol}
H2NCCH2MOH    = 3C + 7H + O  + N      ; {@H2NCCH2MOH}        {2-aminoprop-1-en-1-
ol}

{3C (CHON)}

IPN           = 3C + 7H + 2O + N      ; {@IPN}               {isopropyl nitrite}
CH3CHOCH3     = 3C + 7H + O           ; {@CH3CHOCH3}         {isopropyloxy radical}
MGLYOAC       = 3C + 4H + 3O          ; {@MGLYOAC}           {CH3COCOOH =
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methylglyoxylic acid}

{4C (amines)}

DEA           = 4C + 11H + 2O + N     ; {@DEA}              {diethanolamine}
HOETNETOH     = 4C + 10H + 2O + N     ; {@HOETNETOH}        {N-radical of DEA}
DEAO2         = 4C + 10H + 4O + N     ; {@DEAO2}            {DEA-peroxyradical}
HOETNHCH2CHO  = 4C + 10H + 2O + N     ; {@HOETNHCH2CHO}     {ethanolamine
acetaldehyde}
NDELA         = 4C + 10H + 3O + 2N    ; {@NDELA}            {N-nitroso
diethanolamine}
HOCH2CHNETOH  = 4C + 9H  + 2O + N     ; {@HOCH2CHNETOH}     {DEA imine}
DEANNO2       = 4C + 10H + 4O + 2N    ; {@DEANNO2}          {N-nitro
diethanolamine}
HOCH2CONETOH  = 4C + 8H  + 3O + N     ; {@HOCH2CONETOH}     {ethanol
hydroxyacetamide}
AMP           = 4C + 11H + O + N      ; {@AMP}              {2-amino-2-methyl-1-
propanol}
AMPN          = 4C + 10H + O + N      ; {@AMPN}             {N-radical of AMP}
NAMP          = 4C + 10H + 2O + 2N    ; {@NAMP}             {N-nitroso AMP}
AMPNNO2       = 4C + 10H + 3O + 2N    ; {@AMPNNO2}          {N-nitro AMP}
AMPOX         = 4C + 10H + 2O + N     ; {@AMPOX}            {AMP N-oxide}
DMCNH2CHO     = 4C + 9H + O + N       ; {@DMCNH2CHO}        {2-amino-2-methyl-1-
propanal}
AMPNA         = 4C + 9H + 3O + 2N     ; {@AMPNA}            {N-Nitro-2-amino-2-
methyl-1-propanal}
DMCNH2CO3     = 4C + 8H + 3O + N      ; {@DMCNH2CO3}        {AMP peroxy acetyl
radical}
AMPAN         = 4C + 8H + 5O + 2N     ; {@AMPAN}            {AMP PAN-type
compound}
AMPO          = 4C + 10H + 2O + N     ; {@AMPO}             {AMP alkoxy radical}
DMOCNH2MOH    = 4C + 9H  + 2O + N     ; {@DMOCNH2MOH}       {2-amino-3-hydroxy-2-
methylpropanal}

{5C (amines)}

DEANCHO       = 5C + 11H + 3O + N     ; {@DEANCHO}          {N-diethanol
formamide}
DEANCH2O2     = 5C + 12H + 4O + N     ; {@DEANCH2O2}        {N-diethanol formamide
peroxyradical}

{6C (CHO)}

TME           = 6C + 12H              ; {@TME}              {Tetramethyl ethylene}
TMEO2         = 6C + 13H + 3O         ; {@TMEO2}            {Tetramethyl ethylene
peroxide}
CHEX          = 6C + 12H              ; {@CHEX}             {Cyclohexane}
CHEXO2        = 6C + 11H + 2O         ; {@CHEXO2}           {Cyclohexane
peroxyradical}
CHEXO         = 6C + 11H + O          ; {@CHEXO}            {Cyclohexane
alkoxyradical}
CHEXOL        = 6C + 12H + O          ; {@CHEXOL}           {Cyclohexanol}
CHEXONE       = 6C + 11H + O          ; {@CHEXONE}          {Cyclohexone}
CHEXOOH       = 6C + 12H + 2O         ; {@CHEXOOH}          {Cyclohexane
hydroperoxide}

{6C (amines)}

TEA           = 6C + 15H + 3O + N     ; {@TEA}              {triethanolamin}
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TEAO2          = 6C + 14H + 5O + N     ; {@TEAO2}              {TEA-peroxyradical}
TEAO           = 6C + 14H + 4O + N     ; {@TEAO}               {TEA-alkoxyradical}
DEANCOCH2OH    = 6C + 13H + 4O + N     ; {@DEANCOCH2OH}        {N,N-diethanol
hydroxyacetamide}
DEANCH2CHO     = 6C + 13H + 3O + N     ; {@DEANCH2CHO}         {N,N-diethanol
acetamide}
DEANCH2COO2    = 6C + 12H + 5O + N     ; {@DEANCH2COO2}        {N,N-diethanol
acetamide peroxyradical}



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

HSO3           = S + H + 3O            ; {@HSO_3}              {sulfonic acid}
CH3SOH         = C + 4H + S + O        ; {@CH_3SOH}            {MSEA}
CH3SOOH        = C + 4H + S + 2O       ; {@CH_3SOOH}           {MSIA: methane
sulfinic acid}
CH3SOO2H       = C + 4H + S + 3O       ; {@CH_3SOO_2H}         {}
CH3SO4H        = C + 4H + S + 4O       ; {@CH_3SO_4H}          {}
CH3SCH2        = 2C + 5H + S           ; {@CH_3SCH_2}          {dimethyl sulfide
radical}
DMSOO          = 2C + 5H + S + 2O      ; {@CH_3SCH_2OO}        {dimethyl sulfide
peroxyradical}
DMSOOH         = 2C + 6H + S + 2O      ; {@CH_3SCH_2OOH}       {dimethyl sulfide
hydroperoxide}
DMSOH          = 2C + 7H + S + O       ; {@DMSOH}              {dimethyl
sulfhydroxide: CH3SOHCH3}
DMSOHO         = 2C + 7H + S + 2O      ; {@DMSOHO}             {}
DMSOHOO        = 2C + 7H + S + 3O      ; {@DMSOHOO}            {}
CH3SOCH2       = 2C + 5H + S + O       ; {@CH_3SOCH_2}         {dimethyl sulfoxide
radical}
DMSOOO         = 2C + 5H + S + 3O      ; {@CH_3SOCH_2O_2}      {dimethyl sulfoxide
peroxyradical}
DMSO2          = 2C + 6H + S + 2O      ; {@DMSO_2}             {dimethyl sulfone:
CH3SO2CH3}
DMSO2O         = 2C + 6H + S + 3O      ; {@DMSO_2O}            {dimethyl sulfone
oxyradical}
DMSO2OO        = 2C + 6H + S + 4O      ; {@DMSO_2OO}           {dimethyl sulfone
peroxyradical}
DMSO2OOH       = 2C + 6H + S + 4O      ; {@DMSO_2OOH}          {dimethyl sulfone
hydroperoxide}
CH3S           = C + 3H + S            ; {@CH_3S}              {}
CH3SO          = C + 3H + S + O        ; {@CH_3SO}             {}
CH3SOO         = C + 3H + S + 2O       ; {@CH_3SOO}            {}
CH3SOO2        = C + 3H + S + 3O       ; {@CH_3SOO_2}          {}
CH3SO4         = C + 3H + S + 4O       ; {@CH_3SO_2O_2}        {}
MSON           = C + 3H + S + 4O + N   ; {@CH_3SOONO_2}        {}
MSOON          = C + 3H + S + 5O + N   ; {@CH_3SOO_2NO_2}      {}
MSPN           = C + 3H + S + 6O + N   ; {@CH_3SO_2O_2NO_2}    {methyl sulfonyl
peroxynitrate}
MSAH2O         = C + 7H + S + 4O       ; {@MSA(H_2O)}          {[MSA*H2O]: methane
sulfonic acid - water cluster}
MSADMAH2O      = 3C+ 14H+ S + 4O + N   ; {@MSA(DMA)(H_2O)}     {[MSA*DMA*H2O]:
methane sulfonic acid - DMA - water cluster}
MSADMA         = 3C+ 11H+ S + 3O + N   ; {@MSA(DMA)}           {[MSA*DMA]: methane
sulfonic acid - DMA cluster}
MSATMAH2O      = 4C+ 16H+ S + 4O + N   ; {@MSA(TMA)(H_2O)}     {[MSA*TMA*H2O]:
methane sulfonic acid - TMA - water cluster}
MSATMA         = 4C+ 13H+ S + 3O + N   ; {@MSA(TMA)}           {[MSA*TMA]: methane
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```
sulfonic acid - TMA cluster}

{***** END:   gas-phase species from gas.spc *****}
{**** START: aerosol species (phase 1) from aqueous.spc ****}
{-------------------------------------------------------------------------------}
{------------------------------ aerosol mode: 01 -------------------------------}
{-------------------------------------------------------------------------------}

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

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

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_3OO><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>}
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{peroxyacetylnitrate}
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}

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

SO2_a01        = S + 2O               ; {@\FormatAq<SO_2><01>}         {sulfur
dioxide}
H2SO4_a01      = 2H + S + 4O          ; {@\FormatAq<H_2SO_4><01>}      {sulfuric
acid}
DMS_a01        = 2C + 6H + S          ; {@\FormatAq<DMS><01>}          {dimethyl
sulfide: CH3SCH3}
DMSO_a01       = 2C + 6H + S + O      ; {@\FormatAq<DMSO><01>}         {dimethyl
sulfoxide: CH3SOCH3}

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

Hg_a01         = Hg                   ; {@\FormatAq<Hg><01>}           {mercury}
HgO_a01        = Hg + O               ; {@\FormatAq<HgO><01>}          {}
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HgOHOH_a01     = Hg + 2O + 2H          ; {@\FormatAq<Hg(OH)_2><01>}     {}
HgOHCl_a01     = Hg + O + H + Cl       ; {@\FormatAq<Hg(OH)Cl><01>}     {}
HgCl2_a01      = Hg + 2Cl              ; {@\FormatAq<HgCl_2><01>}       {}
HgBr2_a01      = Hg + 2Br              ; {@\FormatAq<HgBr_2><01>}       {}
HgSO3_a01      = Hg + S + 3O           ; {@\FormatAq<HgSO_3><01>}       {}
ClHgBr_a01     = Hg + Cl + Br          ; {@\FormatAq<ClHgBr><01>}       {}
BrHgOBr_a01    = Hg + O + 2Br          ; {@\FormatAq<BrHgOBr><01>}      {}
ClHgOBr_a01    = Hg + O + Cl + Br      ; {@\FormatAq<ClHgOBr><01>}      {}

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

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

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

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

O2m_a01        = 2O            + Min  ; {@\FormatAq<O_2^-><01>}        {}
OHm_a01        = H +  O        + Min  ; {@\FormatAq<OH^-><01>}         {}
HO2m_a01       = H + 2O        + Min  ; {@\FormatAq<HO2^-><01>}        {}
O2mm_a01       = 2O            + 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       =      2O +  N   + Min ; {@\FormatAq<NO_2^-><01>}       {nitrite}
NO3m_a01       =      3O +  N   + Min ; {@\FormatAq<NO_3^-><01>}       {nitrate}
NO4m_a01       =      4O +  N   + Min ; {@\FormatAq<NO_4^-><01>}       {peroxy
nitrate}

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

{1C}
CO3m_a01       = C + 3O         + Min ; {@\FormatAq<CO_3^-><01>}       {}
HCOOm_a01      = H + C + 2O     + Min ; {@\FormatAq<HCOO^-><01>}       {formate}
HCO3m_a01      = H + C + 3O     + Min ; {@\FormatAq<HCO_3^-><01>}      {hydrogen
carbonate}

{2C}
CH3COOm_a01    = 2C + 3H + 2O   + Min ; {@\FormatAq<CH_3COO^-><01>}    {acetate}

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

Clm_a01        = Cl             + Min ; {@\FormatAq<Cl^-><01>}         {chloride}
Cl2m_a01       = 2Cl            + Min ; {@\FormatAq<Cl_2^-><01>}       {}
ClOm_a01       = Cl + O         + Min ; {@\FormatAq<ClO^-><01>}        {}
ClOHm_a01      = H + O + Cl     + Min ; {@\FormatAq<ClOH^-><01>}       {}

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

Brm_a01        = Br             + Min ; {@\FormatAq<Br^-><01>}         {bromide}
Br2m_a01       = 2Br            + Min ; {@\FormatAq<Br_2^-><01>}       {}
BrOm_a01       = Br + O         + Min ; {@\FormatAq<BrO^-><01>}        {}
```

```
BrOHm_a01      = H + O + 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 + 2O         + Min ; {@\FormatAq<IO_2^-><01>}       {}
IO3m_a01       = I + 3O         + 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 + 3O          + Min ; {@\FormatAq<SO_3^-><01>}       {}
SO3mm_a01      = S + 3O         + 2Min ; {@\FormatAq<SO_3^<2->><01>}    {sulfite}
SO4m_a01       = S + 4O          + Min ; {@\FormatAq<SO_4^-><01>}       {}
SO4mm_a01      = S + 4O         + 2Min ; {@\FormatAq<SO_4^<2->><01>}    {sulfate}
SO5m_a01       = S + 5O          + Min ; {@\FormatAq<SO_5^-><01>}       {}
HSO3m_a01      = H + S + 3O      + Min ; {@\FormatAq<HSO_3^-><01>}      {hydrogen
sulfite}
HSO4m_a01      = H + S + 4O      + Min ; {@\FormatAq<HSO_4^-><01>}      {hydrogen
sulfate}
HSO5m_a01      = H + S + 5O      + Min ; {@\FormatAq<HSO_5^-><01>}      {}
CH3SO3m_a01    = C + 3H + S + 3O + Min ; {@\FormatAq<CH_3SO_3^-><01>}   {MSA anion}
CH2OHSO3m_a01  = C + 3H + S + 4O + 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 + O + 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 + 6O     + 2Min ; {@\FormatAq<Hg(SO_3)_2^<2->><01>}  {}

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

Fepp_a01        = Fe            + 2Pls ; {@\FormatAq<Fe^<2+>><01>}
{Fe(II)}
FeOpp_a01       = Fe + O        + 2Pls ; {@\FormatAq<FeO^<2+>><01>}
{Fe(II)}
FeOHp_a01       = Fe + O + H    + Pls  ; {@\FormatAq<FeOH^+><01>}
{Fe(II)}
FeOH2p_a01      = Fe + 2O + 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)}
FeHOpp_a01      = Fe + O + H    + 2Pls ; {@\FormatAq<FeHO^<2+>><01>}
{Fe(III)}
FeHO2pp_a01     = Fe + 2O + H   + 2Pls ; {@\FormatAq<FeHO_2^<2+>><01>}
{Fe(III)}
FeOHpp_a01      = Fe + O + H    + 2Pls ; {@\FormatAq<FeOH^<2+>><01>}
{Fe(III)}
FeOH4m_a01      = Fe + 4O + 4H  + Min  ; {@\FormatAq<Fe(OH)_4^-><01>}
{Fe(III)}
FeOHHO2p_a01    = Fe + 3O + 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)}
FeSO3p_a01      = Fe + 3O + S    + Pls  ; {@\FormatAq<FeSO_3^+><01>}
{Fe(III)}
FeSO4p_a01      = Fe + 4O + S    + Pls  ; {@\FormatAq<FeSO_4^+><01>}
{Fe(III)}
FeSO42m_a01     = Fe + 8O + 2S   + Min  ; {@\FormatAq<Fe(SO_4)_2^-><01>}
{Fe(III)}
FeOH2Fepppp_a01 = 2 Fe + O + H   + 4Pls ; {@\FormatAq<Fe(OH)_2Fe^<4+>><01>}
{Fe(III)}

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

D1O_a01         = Ignore              ; {@\FormatAq<D_1O><01>}         {}
Nap_a01         = Ignore              ; {@\FormatAq<Na^+><01>}         {dummy
cation}
{-------------------------------------------------------------------------------}
{------------------------------ aerosol mode: 01 -------------------------------}
{-------------------------------------------------------------------------------}

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

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

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

{------------------------------------ N ------------------------------------}
N2O3_a01        =              3O  + 2N  ; {@\FormatAq<N_2O_3><01>}
{dinitrogen trioxide}
N2O4_a01        =              4O  + 2N  ; {@\FormatAq<N_2O_4><01>}
{dinitrogen tetraoxide}

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

{1C}
CH2O2H2_a01     =   C +  4H +  2O        ; {@\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 +   O  +  N  ; {@\FormatAq<HNCO><01>}
{ioscyanic acid}
H2NCHO_a01      =   C +  3H +   O  +  N  ; {@\FormatAq<H2NCHO><01>}
{formamide}
MMNNO2_a01      =   C +  2H +  2O  + 2N  ; {@\FormatAq<MMNNO2><01>}
{methylnitramine}
```

```
{2C}
OXALAC_a01     =  IGNORE               ; {@\FormatAq<OXALAC><01>}          {oxalic
acid, 2C +  2H  +  4O}
HCOCO2H_a01    =  2C +  2H  +  3O      ; {@\FormatAq<HCOCO_2H><01>}
{oxoethanoic acid}
HOCH2CHO_a01   =  2C +  4H  +  2O      ; {@\FormatAq<HOCH_2CHO><01>}
{glycolaldehyde}
HOCH2CO2H_a01  =  2C +  4H  +  3O      ; {@\FormatAq<HOCH_2CO_2H><01>}
{hydroxyethanoic acid}
CH3CO3_a01     =  2C +  3H  +  3O      ; {@\FormatAq<CH_3COO_2><01>}
{peroxyacetyl radical}
GLYOX_a01      =  2C +  2H  +  2O      ; {@\FormatAq<GLYOX><01>}           {CHOCHO
= glyoxal}
DMA_a01        =  2C +  7H        +  N ; {@\FormatAq<DMA><01>}
{dimethylamine}
MEA_a01        =  2C +  7H  +   O  +  N ; {@\FormatAq<MEA><01>}
{ethanolamine}
MEANNO_a01     =  2C +  6H  +  2O  + 2N ; {@\FormatAq<MEANNO><01>}          {N-
nitroso ethanolamine}
MEANNO2_a01    =  2C +  6H  +  3O  + 2N ; {@\FormatAq<MEANNO2><01>}         {N-
nitro ethanolamine}
NDMA_a01       =  2C +  6H  +   O  + 2N ; {@\FormatAq<NDMA><01>}            {N-
nitroso dimethylamine}
DMNNO2_a01     =  2C +  6H  +  2O  + 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  +   O  +  N ; {@\FormatAq<NH_2CH_2CHOH><01>}
{ethanolamine radical}
H2NCOCH2OH_a01 =  2C +  5H  +  2O  +  N ; {@\FormatAq<H2NCOCH2OH><01>}      {2-
hydroxy acetamide}
CH3NHCHO_a01   =  2C +  5H  +   O  +  N ; {@\FormatAq<CH_3NHCHO><01>}       {N-
methyl formamide}
CH3NCO_a01     =  2C +  3H  +   O  +  N ; {@\FormatAq<CH_3NCO><01>}         {methyl
isocyanic acid}

{3C}
MGLYOX_a01     =  3C +  4H  +  2O      ; {@\FormatAq<MGLYOX><01>}
{methylglyoxal}
MGLYOAC_a01    =  3C +  4H  +  3O      ; {@\FormatAq<MGLYOAC><01>}
{methylglyoxylic acid}
DOC_a01        =  IGNORE               ; {@\FormatAq<DOC><01>}
{dissolved organic carbon DOC}
DOCO_a01       =  IGNORE               ; {@\FormatAq<DOCO><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  +   O  +  N ; {@\FormatAq<DMNCHO><01>}          {N,N-
dimethyl formamide}
MALONAC_a01    =  IGNORE               ; {@\FormatAq<MALONAC><01>}
{malonic acid, 3C +  4H  +  4O}
```

```
{4C}
DEA_a01        =  4C + 11H  +  2O  +  N ; {@\FormatAq<DEA><01>}
{diethanolamine}
NDELA_a01      =  4C + 10H  +  3O  + 2N ; {@\FormatAq<NDELA><01>}           {N-
nitroso diethanolamine}
DEANNO2_a01    =  4C + 10H  +  4O  + 2N ; {@\FormatAq<DEANNO2><01>}         {N-
nitro diethanolamine}
DEAN_a01       =  4C + 10H  +  2O  +  N ; {@\FormatAq<HOETNHCH_2CHOH><01>}
{diethanolamine radical}
SUCCAC_a01     =  IGNORE               ; {@\FormatAq<SUCCAC><01>}
{succinic acid, 4C +  6H  +  4O}

{5C}
GLUTARAC_a01   =  IGNORE               ; {@\FormatAq<GLUTARAC><01>}
{glutaric acid, 5C +  8H  +  4O}

{6C}
TEA_a01        =  6C + 15H  +  3O  +  N ; {@\FormatAq<TEA><01>}
{triethanolamine}
DENCH2CHOH_a01 =  6C + 14H  +  3O  +  N ; {@\FormatAq<DENCH_2CHOH><01>}
{triethanolamine radical}
ADIPAC_a01     =  IGNORE               ; {@\FormatAq<ADIPAC><01>}          {adipic
acid, 6C + 10H  +  4O}


{----------------------------------- 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        +   O  +  N  + Min  ; {@\FormatAq<NCO^-><01>}
{isocyanate}


{2C}
HC2O4m_a01     =  IGNORE                + Min  ; {@\FormatAq<HC_2O_4^-><01>}
{hydrogen oxalate,2C +   H  +  4O}
C2O4mm_a01     =  IGNORE                + 2Min ; {@\FormatAq<C_2O_4^<2->><01>}
{oxalate, 2C        +  4O}
HCOCOOm_a01    =  2C +   H  +  3O       + Min  ; {@\FormatAq<HCOCOO^-><01>}
{}
MEAp_a01       =  2C +  8H  +   O  +  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  +   O  +  N  + Pls  ; {@\
FormatAq<HOCH_2CH_2NH_2^+><01>}  {ethanolamine N-radical cation}
NH3CH2CHOHp_a01 = 2C +  7H  +   O  +  N  + Pls  ; {@\FormatAq<HOCHCH_2NH_3^+><01>}
{ethanolaminium radical}

{3C}
CH3COCOOm_a01  =  3C +  3H   + 3O        + Min  ; {@\FormatAq<CH_3COCOO^-><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)_2N^+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  +  2O  +  N  + Pls  ; {@\FormatAq<DEA^+><01>}
{diethanolaminium}
DENp_a01       =  4C + 13H  +  2O  +  N  + Pls  ; {@\FormatAq<(HOET)_2NH^+><01>}
{diethanolamine N-radical cation}
DENHp_a01      =  4C + 12H  +  2O  +  N  + Pls  ; {@\
FormatAq<HOETNH_2CH_2CHOH^+><01>}   {diethanolaminium radical}
C2H5C2O4m_a01  =  IGNORE                + Min  ; {@\FormatAq<CH_2CH_2HC_2O_4^-
><01>}    {hydrogen succinate, 4C +  5H  +  4O}
C2H4C2O4mm_a01 =  IGNORE                + 2Min ; {@\FormatAq<CH_2CH_2C_2O_4^<2-
>><01>}  {succinate, 4C +  4H  +  4O}

{6C}
TEAp_a01       =  6C + 16H  +  3O  +  N  + Pls ; {@\FormatAq<TEA^+><01>}
{triethanolaminium}
TENp_a01       =  6C + 15H  +  3O  +  N  + Pls ; {@\FormatAq<(HOET)_3N^+><01>}
{triethanolamine N-radical cation}
DENIMp_a01     =  6C + 15H  +  3O  +  N  + Pls ; {@\
FormatAq<(HOET)_2N^+CH_2CH_2OH><01>} {diethanol iminium}
TENHp_a01      =  6C + 15H  +  3O  +  N  + Pls ; {@\
FormatAq<(HOET)_2NH^+CH_2CHOH><01>}  {triethanolaminium radical}


{-------------------------------------M----------------------------------------}
{**** END:   aerosol species (phase 1) from aqueous.spc ****}
{SETFIX H2O_a* is done via xmecca}
#SETFIX H2O_a01;
```