
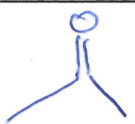
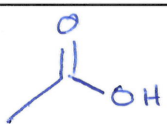


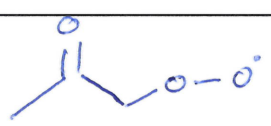
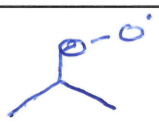









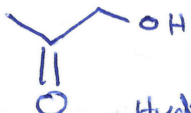
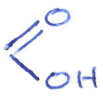
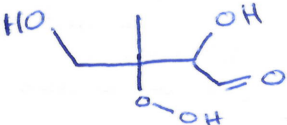
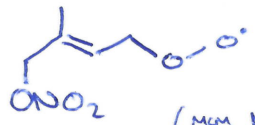
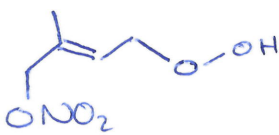
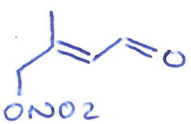
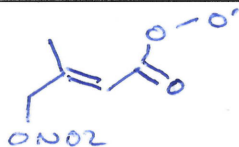


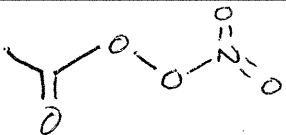
Species	Structure	Comments
A3O2	 <chem>CCCO[O]</chem>	MCM - NC3H7O2
ACET	 <chem>CC(=O)C</chem> acetone	CH3COCH3
ACTA	 <chem>CC(=O)O</chem> Acetic acid	CH3CO2H
ALD2	 <chem>CC=O</chem> Acetaldehyde	CH3CHO
ALK4	 <chem>CCCC</chem> n-butane	NC4H10
ATO2	 <chem>CC(=O)CO[O]</chem>	CH3COCH2O2
B3O2	 <chem>CCCO[O]</chem>	1C3H7O2
C2H6	 <chem>CC</chem> Ethane	C2H6
C3H8	 <chem>CCC</chem> Propane	C3H8
CH2O	 <chem>C=O</chem> formaldehyde	HCHO
CH4	 <chem>CH4</chem> methane	CH4


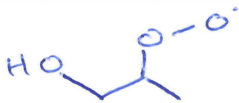
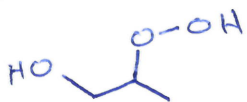
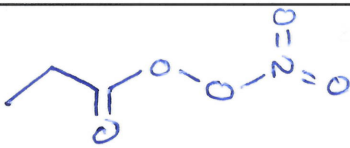
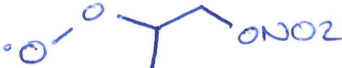


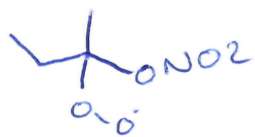
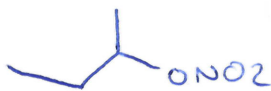
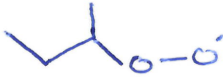
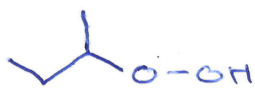
CO		
CO ₂		
EOH	 ethanol	C ₂ H ₅ OH
ETO ₂	 ethanoate	C ₂ H ₅ O ₂ ⁻
ETP	 ethanoyl peroxide	C ₂ H ₅ OOH
GLYC	 Glyceraldehyde	HOCH ₂ CHO
GLYX	 Glyoxal	GLYOX
H		
H ₂		
H ₂ O		
H ₂ O ₂		


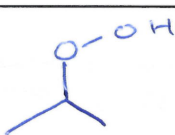
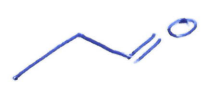
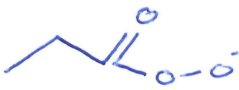
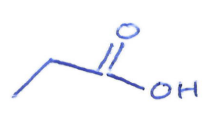
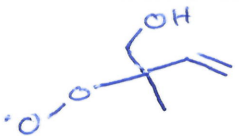



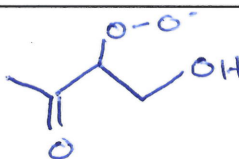
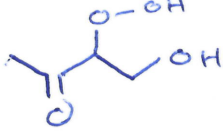
HAC	 Hydroxyacetone	ACETOL
HCOOH	 Formic acid	HCOOH
HNO2		
HNO3		
HNO4		
HO2		
IAP		
INO2	 (Mem NISOP02)	The wiki references Paulot for the isop stuff. In Paulot 2009 & Mao 2013 they use Rollins 09. The structure (left) is from Rollins 09 this does not match the formula given on the wiki.
INPN		NISOP00H See INO2
ISN1		NC4CHO See INO2
ISNOOA		NC4CO3 See INO2


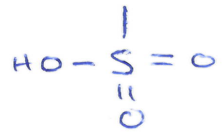
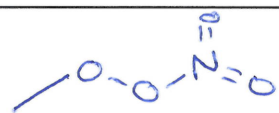
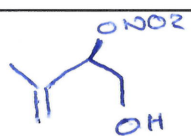
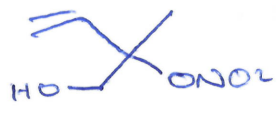
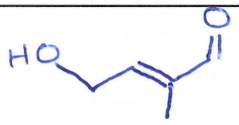
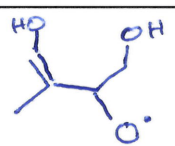

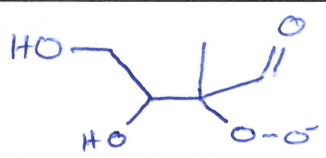
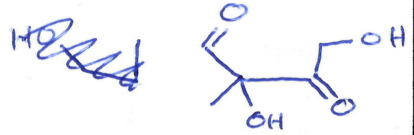
ISNOOB	<p>NO₃ adds to C=C in ISNI</p>	<p>This is most one of my least confident allocations as there is no description on the wiki. It does however match NIT3 from Rollins et al 09 & the production rxn & most of the reactions of this species make sense with this structure</p>
ISNOHOO	<p>OH adds to C=C in ISNI</p>	CS1002
ISNP		INDOOH
ISOP		CSH8
KO2		MEKBO2
MACR		MACR
MAN2		<p>Structure on Wiki is wrong, as is an RO2 from MACR + NO₃ with addition to double bond. Could have positions of group backwards, but this makes most sense for products.</p>
MAO3		MACO3
MAOP		MACO3H
MAOPO2		
MAP	<p>peroxyacetic acid</p>	CH3CO3H

MC03		CH ₃ CO ₃
MEK		MEK
MGLY		MGLYOX
MNO3		CH ₃ NO ₃
MO2		CH ₃ O ₂
MOH	 methanol	CH ₃ OH
MP	 methyl peroxide	CH ₃ OOH
MRO2		MACRO ₂ RO ₂ from MACR + OH
MRP		MACROOH
MVK		
N2O5		

NH ₂		
NH ₃		
NO		
NO ₂		
NO ₃		
O		
O ₁ D		
O ₂		
O ₃		
OH		
PAN		

PMN		MPAN
PO2		HYPROPO2 wiki says this is from isoprene, it's not the from C3 alkene PRPE
PP		HYPROPO2H
PPN		
PRN1		PRONO3BO2
PRPE		C3H6
PRPN		PR2O2HNO3
R4N1		The production of this RO2 from R4NO2 is not in MCM, but this structure makes most sense with reactions
R4N2		SC4H9NO3 This is a highly lumped group. Have called it the product from ALK4, but as described in M&O 2013 this is a large group
R4O2		SC4H9O2
R4P		SC4H9OOH

RA3P		NC3H7OOH
RB3P		IC3H7OOH
RCHO	 Propanal	C2H5CHO
RCO3		C2H5CO3
RCOOH	 Propionic acid Propionic acid	PERPROACID PROPACID
RIO2		ISOPO2
RIP		ISOPOOH
ROH		NPROPOL
RP		PERPROACID
VRO2		HMVK3O2
VRP		HMVK3OOH

DMS		DMS
SO2		
SO4		
MSA		MSA
MPN		CH3O2NO2
ISOPND		ISOPND ISOPDNO3
ISOPNB		ISOPBNO3
HC5		HC4CCHO
DIBOO		
HC500		 C5702
DHMOB		Paulot et al 2009 (fig.1)

MOBA		Paulot et al 2009 (Fig.1)
MOBAOO		
ISOPNBO2		INBIO2
ISOPNDO2		INDO2
PROPNN		
ETHLN		
MACRN		Mao et al (2013)
MVKN		Have gone with structure from Mao et al (2013) as this makes more sense than the formula on the wiki.
PYAC	 Pyruvic acid	CH ₃ COCO ₂ H
IEPOX		IEPOXB Have assigned this the β structure as is dominant channel.
IEPOXOO		IEBIO2 This has multiple 2 possible structures depending on ring opening, in MEM these are 50:50 split.

ATOOH		HYPERALET
PMNN		MACRPAN
MACRNO2		MACRNC03

