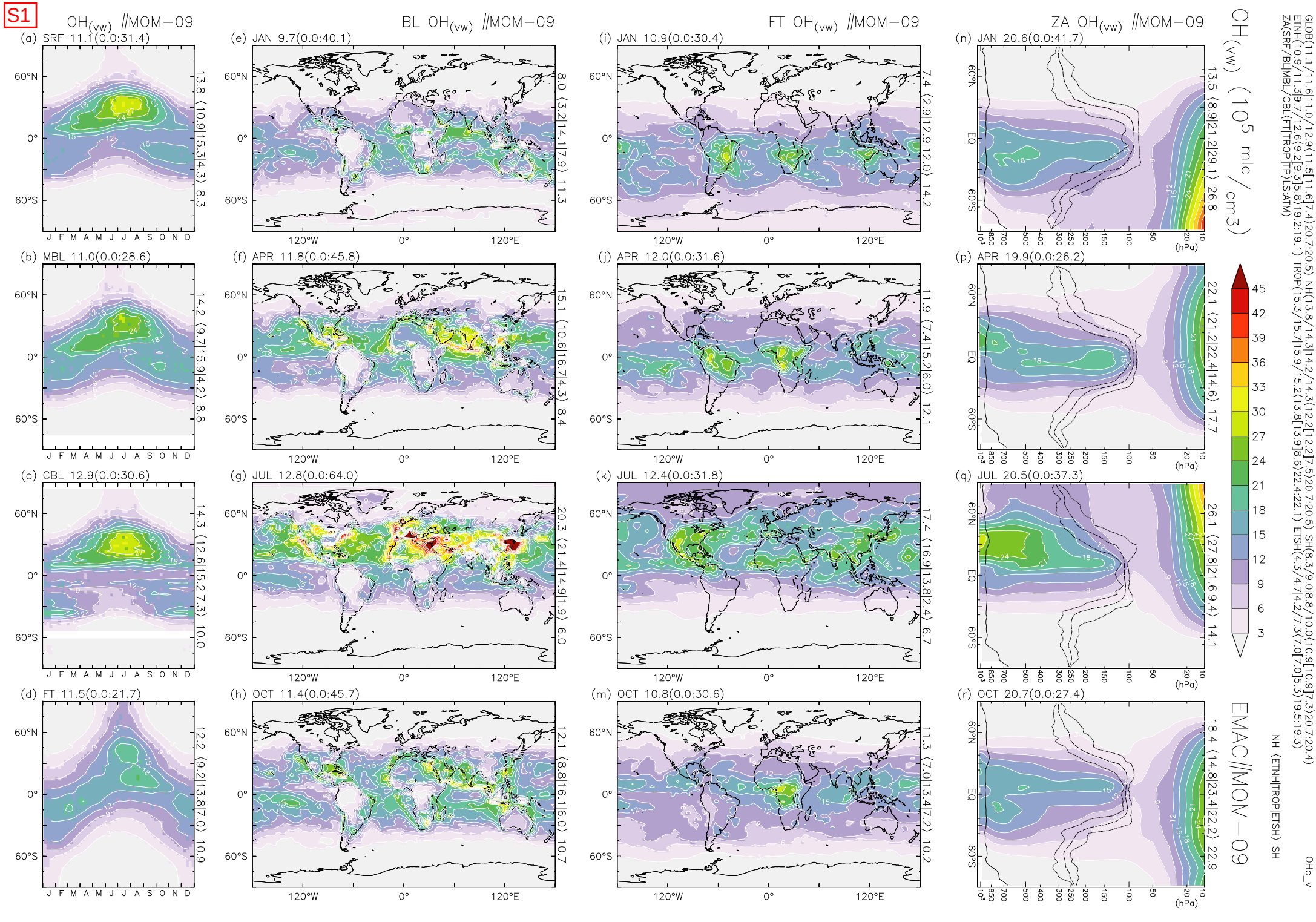
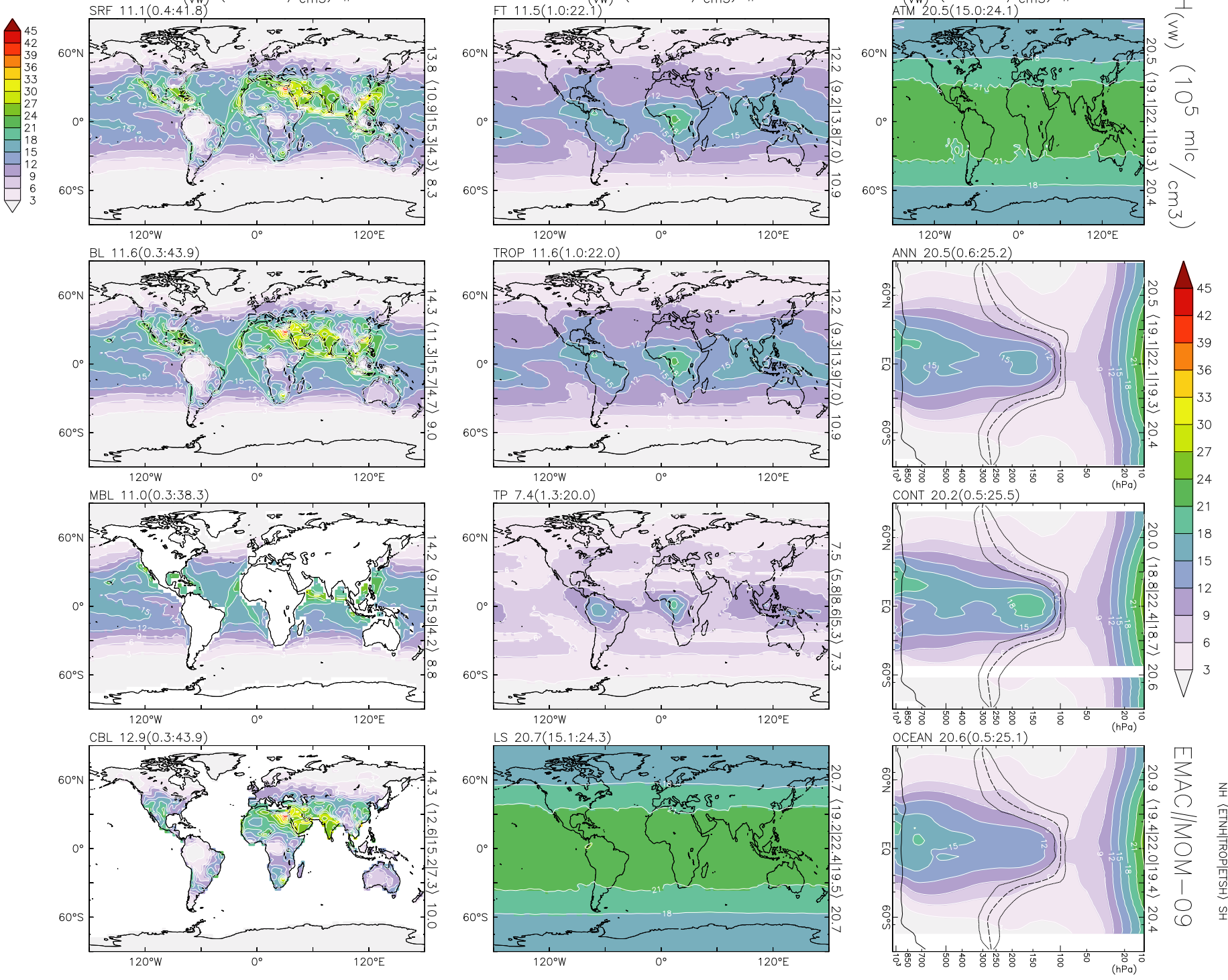
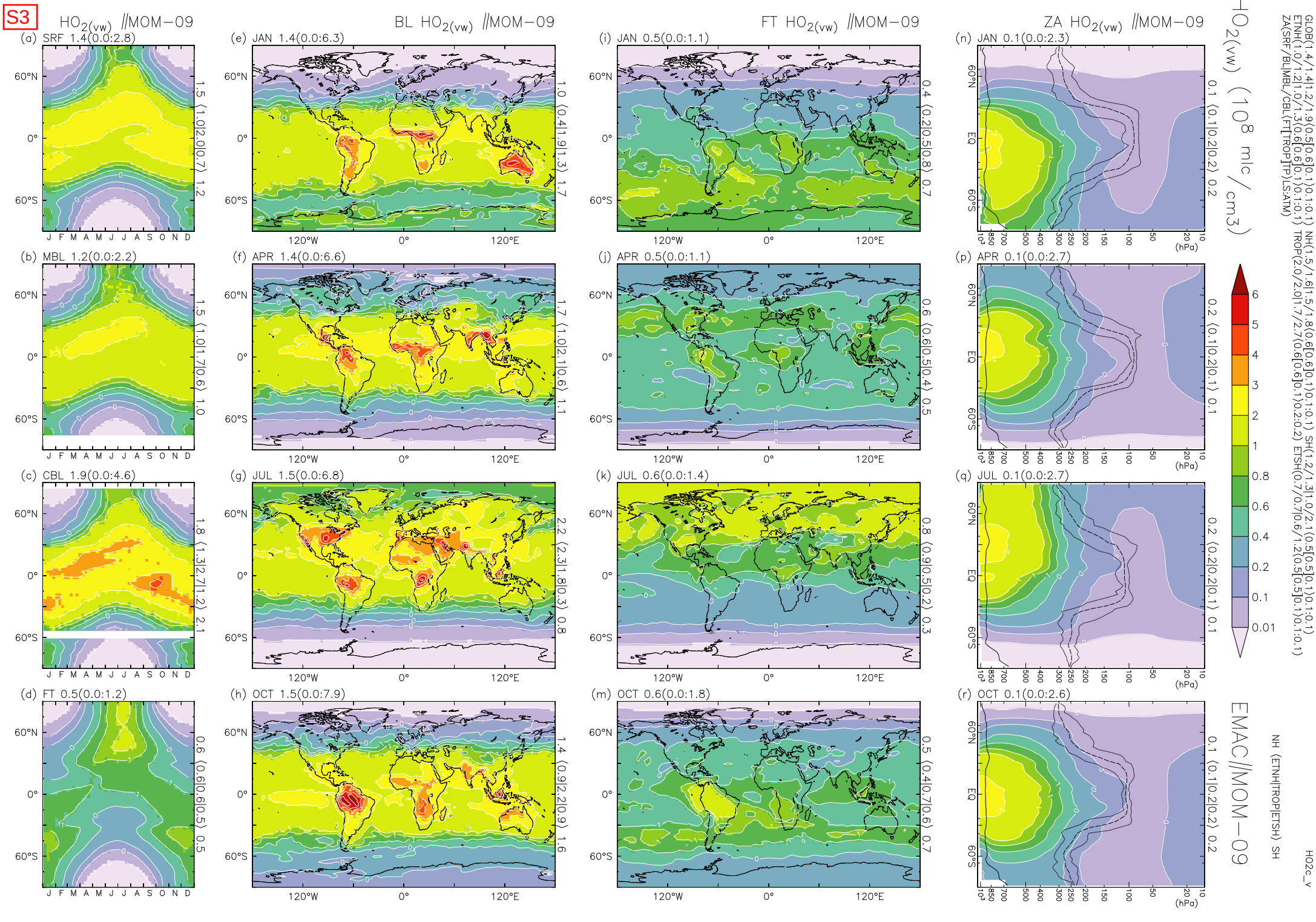
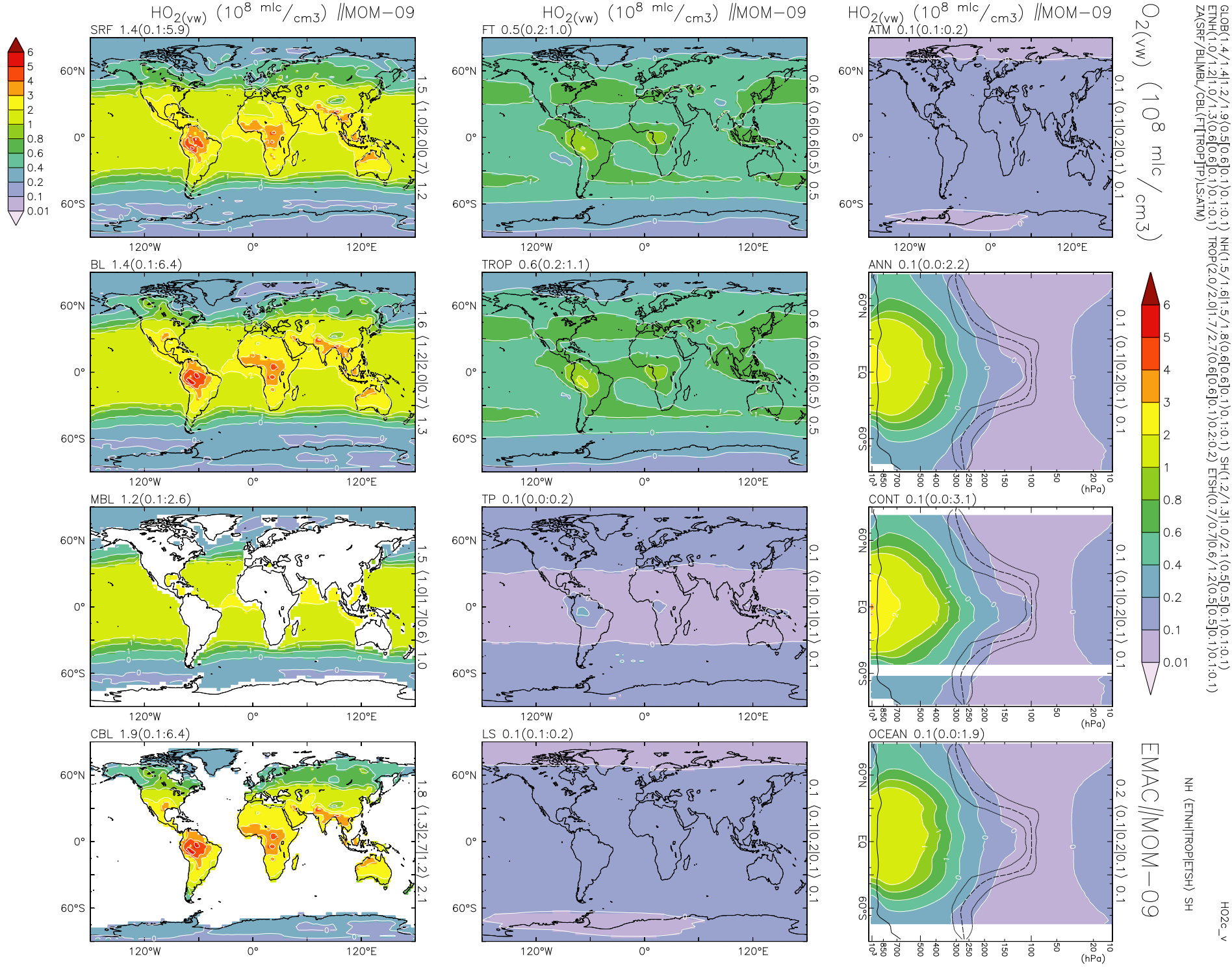

S1
OH(vw) //MOM−09
BL OH(vw) //MOM−09
FT OH(vw) //MOM−09
ZA OH(vw) //MOM−09
(a) SRF 11.1(0.0:31.4)
(b) MBL 11.0(0.0:28.6)
(c) CBL 12.9(0.0:30.6)
(d) FT 11.5(0.0:21.7)
(e) JAN 9.7(0.0:40.1)
(f) APR 11.8(0.0:45.8)
(g) JUL 12.8(0.0:64.0)
(h) OCT 11.4(0.0:45.7)
(i) JAN 10.9(0.0:30.4)
(j) APR 12.0(0.0:31.6)
(k) JUL 12.4(0.0:31.8)
(m) OCT 10.8(0.0:30.6)
(n) JAN 20.6(0.0:41.7)
(p) APR 19.9(0.0:26.2)
(q) JUL 20.5(0.0:37.3)
(r) OCT 20.7(0.0:27.4)
13.8 ⟨10.9|15.3|4.3⟩ 8.3
14.2 ⟨9.7|15.9|4.2⟩ 8.8
14.3 ⟨12.6|15.2|7.3⟩ 10.0
12.2 ⟨9.2|13.8|7.0⟩ 10.9
8.0 ⟨3.2|14.1|7.9⟩ 11.3
15.1 ⟨10.6|16.7|4.3⟩ 8.4
20.3 ⟨21.4|14.9|1.9⟩ 6.0
12.1 ⟨8.8|16.1|6.0⟩ 10.7
7.4 ⟨2.9|12.9|12.0⟩ 14.2
11.9 ⟨7.4|15.2|6.0⟩ 12.1
17.4 ⟨16.9|13.8|2.4⟩ 6.7
11.3 ⟨7.0|13.4|7.2⟩ 10.2
13.5 ⟨8.9|21.2|29.1⟩ 26.8
22.1 ⟨21.2|22.4|14.6⟩ 17.7
26.1 ⟨27.8|21.6|9.4⟩ 14.1
18.4 ⟨14.8|23.4|22.2⟩ 22.9
J F M A M J J A S O N D
60°N
0°
60°S
120°W
0°
120°E
EQ
10³ 850 700 500 400 300 250 200 150 100 50 20 10
(hPa)
OH(vw) (10⁵ mlc / cm3)
45 42 39 36 33 30 27 24 21 18 15 12 9 6 3
EMAC //MOM−09
GLOB(11.1/11.6|11.0/12.9(11.5|11.6|7.4)20.7:20.5) NH(13.8/14.3|14.2/14.3(12.2|12.2|7.5)20.7:20.5) SH(8.3/9.0|8.8/10.0(10.9|10.9|7.3|20.7:20.4)
ETNH(10.9/11.3|9.7/12.6(9.2|9.3|5.8|19.2:19.1) TROP(15.3/15.7|15.9/15.2(13.8|13.9|8.6)22.4:22.1) ETSH(4.3/4.7|4.2/7.3(7.0|7.0|5.3|19.5:19.3)
ZA(SRF/BL/MBL/CBL(FT|TROP|TP)LS:ATM)
NH ⟨ETNH|TROP|ETSH⟩ SH
OHc_v

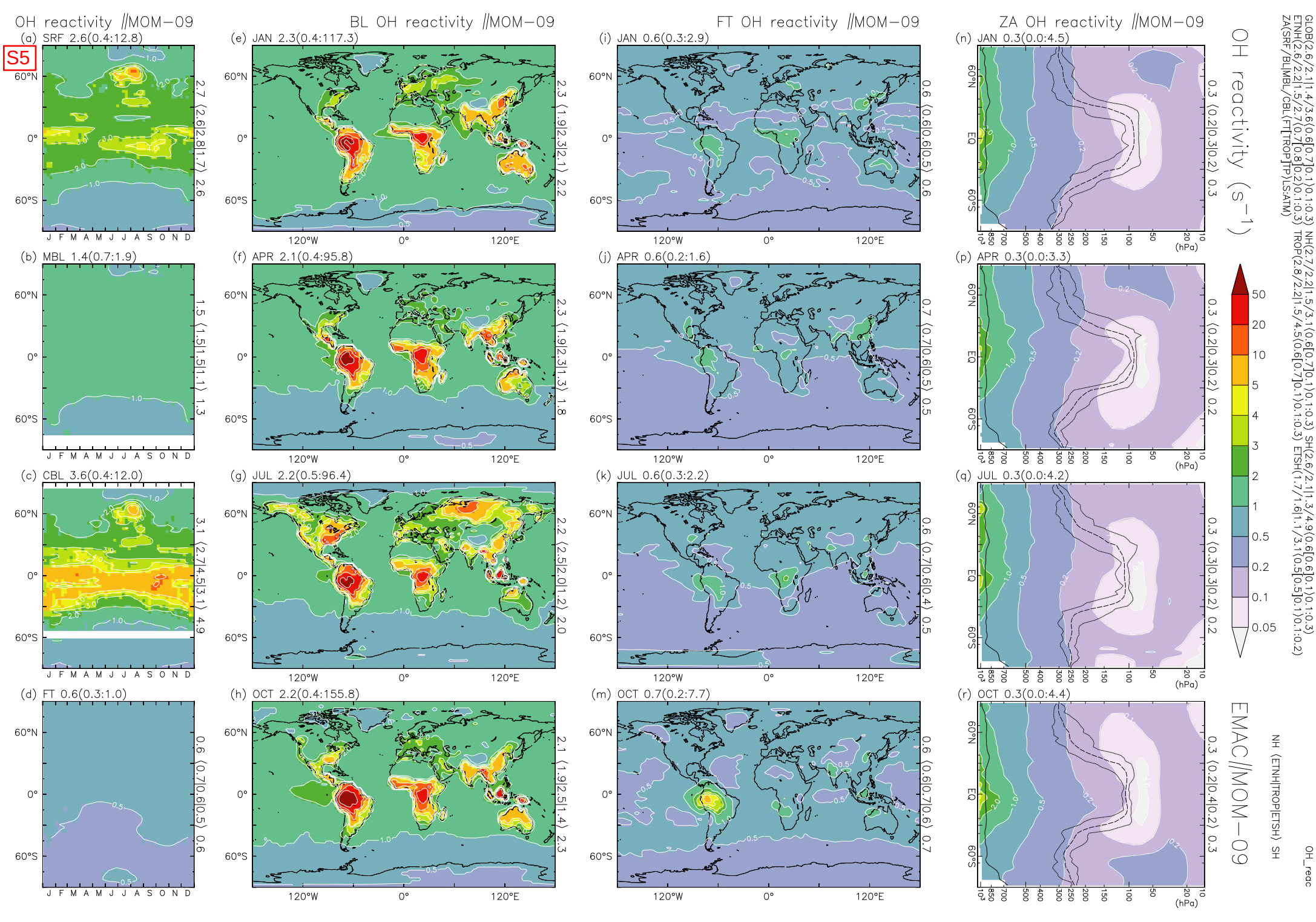
S2


OH(vw) (10^5 mlc/cm3) //MOM-09
SRF 11.1(0.4:41.8)
FT 11.5(1.0:22.1)
ATM 20.5(15.0:24.1)
BL 11.6(0.3:43.9)
TROP 11.6(1.0:22.0)
ANN 20.5(0.6:25.2)
MBL 11.0(0.3:38.3)
TP 7.4(1.3:20.0)
CONT 20.2(0.5:25.5)
CBL 12.9(0.3:43.9)
LS 20.7(15.1:24.3)
OCEAN 20.6(0.5:25.1)
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
45 42 39 36 33 30 27 24 21 18 15 12 9 6 3
OH(vw) (10^5 mlc/cm3)
EMAC //MOM-09
13.8 ⟨10.9|15.3|14.3⟩ 8.3
12.2 ⟨9.2|13.8|7.0⟩ 10.9
20.5 ⟨19.1|22.1|19.3⟩ 20.4
14.3 ⟨11.3|15.7|14.7⟩ 9.0
12.2 ⟨9.3|13.9|7.0⟩ 10.9
20.5 ⟨19.1|22.1|19.3⟩ 20.4
14.2 ⟨9.7|15.9|14.2⟩ 8.8
7.5 ⟨5.8|8.6|5.3⟩ 7.3
20.0 ⟨18.8|22.4|18.7⟩ 20.6
14.3 ⟨12.6|15.2|7.3⟩ 10.0
20.7 ⟨19.2|22.4|19.5⟩ 20.7
20.9 ⟨19.4|22.0|19.4⟩ 20.4
GLOB(11.1/11.6|11.0/12.9(11.5|11.6|7.4)20.7:20.5) NH(13.8/14.3|14.2/14.3(12.2|12.2|7.5)20.7:20.5) SH(8.3/9.0|8.8/10.0(10.9|10.9|7.3)20.7:20.4)
ETNH(10.9/11.3|9.7/12.6(9.2|9.3|5.8)19.2:19.1) TROP(15.3/15.7|15.9/15.2(13.8|13.9|8.6)22.4:22.1) ETSH(4.3/4.7|4.2/7.3(7.0|7.0|5.3)19.5:19.3)
ZA(SRF/BL|MBL/CBL(FT|TROP|TP)LS:ATM)
NH ⟨ETNH|TROP|ETSH⟩ SH
OHc_v

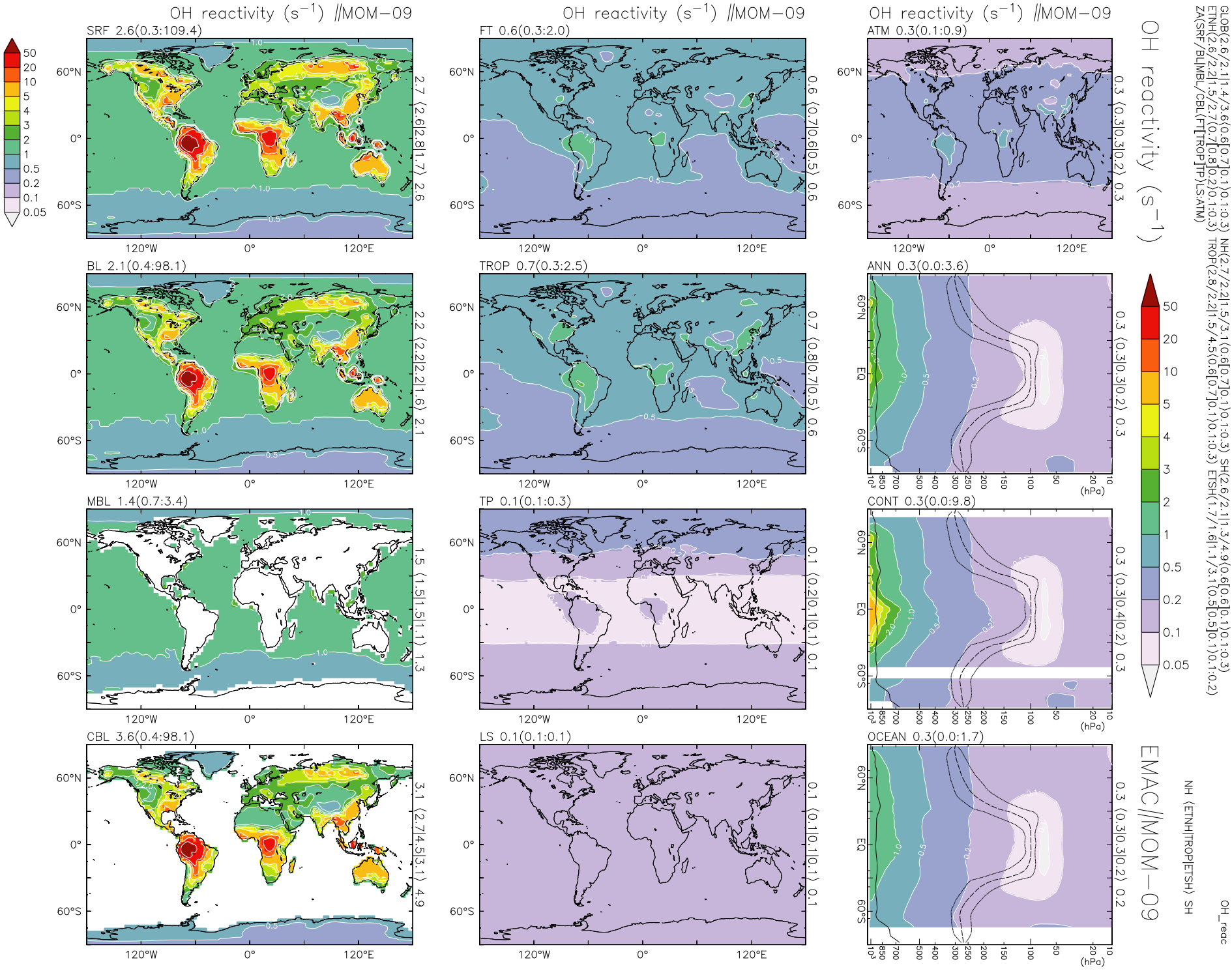

S3
HO2(vw) //MOM−09
BL HO2(vw) //MOM−09
FT HO2(vw) //MOM−09
ZA HO2(vw) //MOM−09
HO2(vw) (10^8 mlc / cm3)
EMAC//MOM−09
(a) SRF 1.4(0.0:2.8)
(b) MBL 1.2(0.0:2.2)
(c) CBL 1.9(0.0:4.6)
(d) FT 0.5(0.0:1.2)
(e) JAN 1.4(0.0:6.3)
(f) APR 1.4(0.0:6.6)
(g) JUL 1.5(0.0:6.8)
(h) OCT 1.5(0.0:7.9)
(i) JAN 0.5(0.0:1.1)
(j) APR 0.5(0.0:1.1)
(k) JUL 0.6(0.0:1.4)
(m) OCT 0.6(0.0:1.8)
(n) JAN 0.1(0.0:2.3)
(p) APR 0.1(0.0:2.7)
(q) JUL 0.1(0.0:2.7)
(r) OCT 0.1(0.0:2.6)
GLOB(1.4/1.4|1.2/1.9(0.5[0.6]0.1)0.1:0.1) NH(1.5/1.6|1.5/1.8(0.6[0.6]0.1)0.1:0.1) SH(1.2/1.3|1.0/2.1(0.5[0.5]0.1)0.1:0.1)
ETNH(1.0/1.2|1.0/1.3(0.6[0.6]0.1)0.1:0.1) TROP(2.0/2.0|1.7/2.7(0.6[0.6]0.1)0.2:0.2) ETSH(0.7/0.7|0.6/1.2(0.5[0.5]0.1)0.1:0.1)
ZA(SRF/BLMBL/CBL(FT[TROP]TP)LS:ATM)
NH ⟨ETNH|TROP|ETSH⟩ SH
HO2c_v

S4

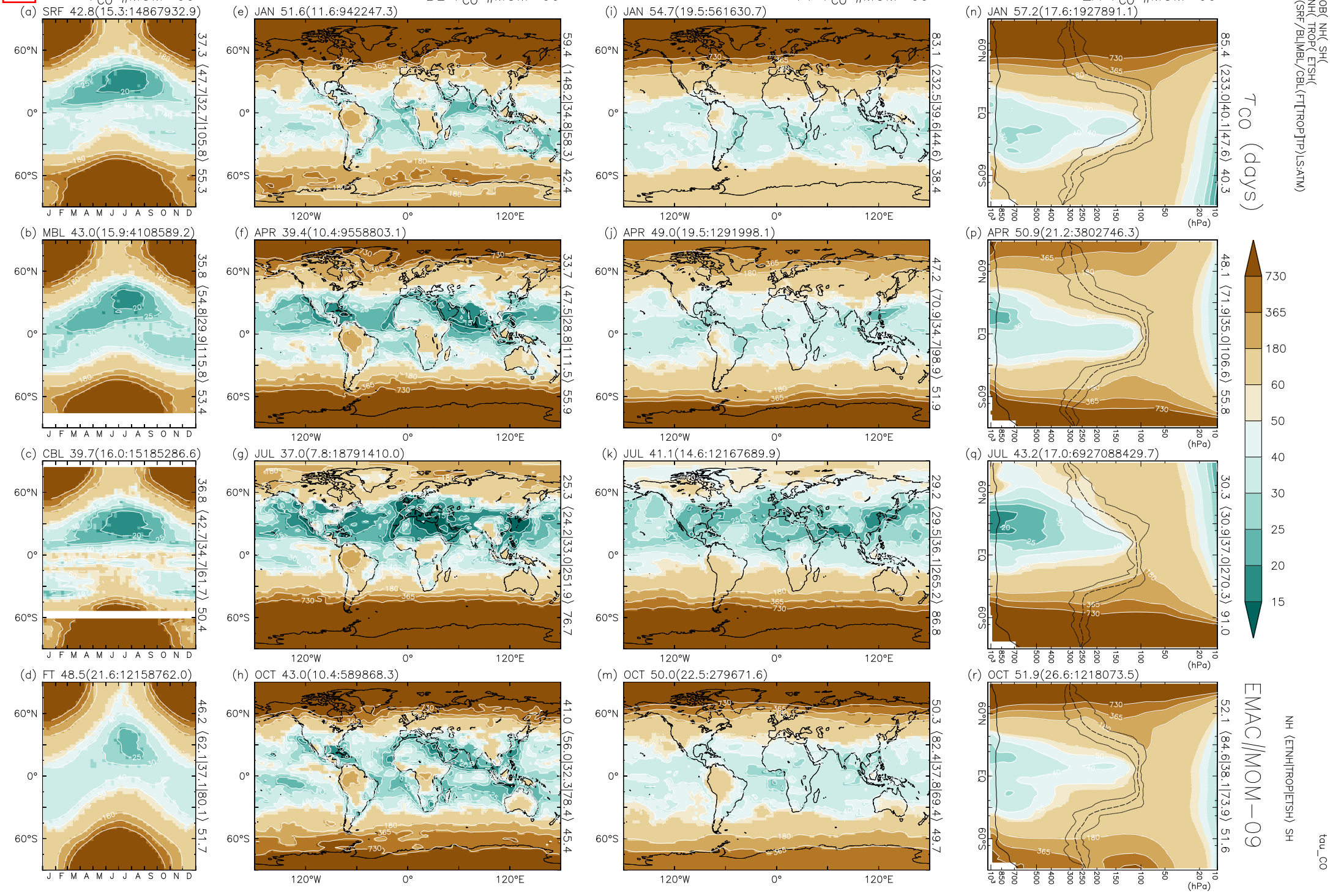

HO2(vw) (10^8 mlc/cm3) //MOM-09
SRF 1.4(0.1:5.9)
FT 0.5(0.2:1.0)
ATM 0.1(0.1:0.2)
BL 1.4(0.1:6.4)
TROP 0.6(0.2:1.1)
ANN 0.1(0.0:2.2)
MBL 1.2(0.1:2.6)
TP 0.1(0.0:0.2)
CONT 0.1(0.0:3.1)
CBL 1.9(0.1:6.4)
LS 0.1(0.1:0.2)
OCEAN 0.1(0.0:1.9)
6
5
4
3
2
1
0.8
0.6
0.4
0.2
0.1
0.01
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
HO2(vw) (10^8 mlc / cm3)
EMAC //MOM-09
NH (ETNH|TROP|ETSH) SH
GLOB(1.4/1.4|1.2/1.9(0.5[0.6]0.1)0.1:0.1) NH(1.5/1.6|1.5/1.8(0.6[0.6]0.1)0.1:0.1) SH(1.2/1.3|1.0/2.1(0.5[0.5]0.1)0.1:0.1)
ETNH(1.0/1.2|1.0/1.3(0.6[0.6]0.1)0.1:0.1) TROP(2.0/2.0|1.7/2.7(0.6[0.6]0.1)0.2:0.2) ETSH(0.7/0.7|0.6/1.2(0.5[0.5]0.1)0.1:0.1)
ZA(SRF/BL|MBL/CBL(FT|TROP|TP)LS:ATM)
HO2c_v


OH reactivity //MOM-09
BL OH reactivity //MOM-09
FT OH reactivity //MOM-09
ZA OH reactivity //MOM-09
S5
(a) SRF 2.6(0.4:12.8)
(b) MBL 1.4(0.7:1.9)
(c) CBL 3.6(0.4:12.0)
(d) FT 0.6(0.3:1.0)
(e) JAN 2.3(0.4:117.3)
(f) APR 2.1(0.4:95.8)
(g) JUL 2.2(0.5:96.4)
(h) OCT 2.2(0.4:155.8)
(i) JAN 0.6(0.3:2.9)
(j) APR 0.6(0.2:1.6)
(k) JUL 0.6(0.3:2.2)
(m) OCT 0.7(0.2:7.7)
(n) JAN 0.3(0.0:4.5)
(p) APR 0.3(0.0:3.3)
(q) JUL 0.3(0.0:4.2)
(r) OCT 0.3(0.0:4.4)
OH reactivity (s⁻¹)
50
20
10
5
4
3
2
1
0.5
0.2
0.1
0.05
EMAC //MOM-09
OH_reac
GLOB⟨2.6/2.1|1.4/3.6⟩(0.6[0.7[0.1⟩0.1:0.3⟩ NH⟨2.7/2.2|1.5/3.1⟩(0.6[0.7[0.1⟩0.1:0.3⟩ TROP⟨2.8/2.2|1.5/4.5⟩(0.6[0.7[0.1⟩0.1:0.3⟩ SH⟨2.6/2.1|1.3/4.9⟩(0.6[0.6[0.1⟩0.1:0.3⟩
ETNH⟨2.6/2.2|1.5/2.7⟩(0.7[0.8[0.2⟩0.1:0.3⟩ ETSH⟨1.7/1.6|1.1/3.1⟩(0.5[0.5[0.1⟩0.1:0.2⟩
ZA(SRF/BL|MBL/CBL(FT|TROP|TP)LS:ATM)
NH ⟨ETNH|TROP|ETSH⟩ SH

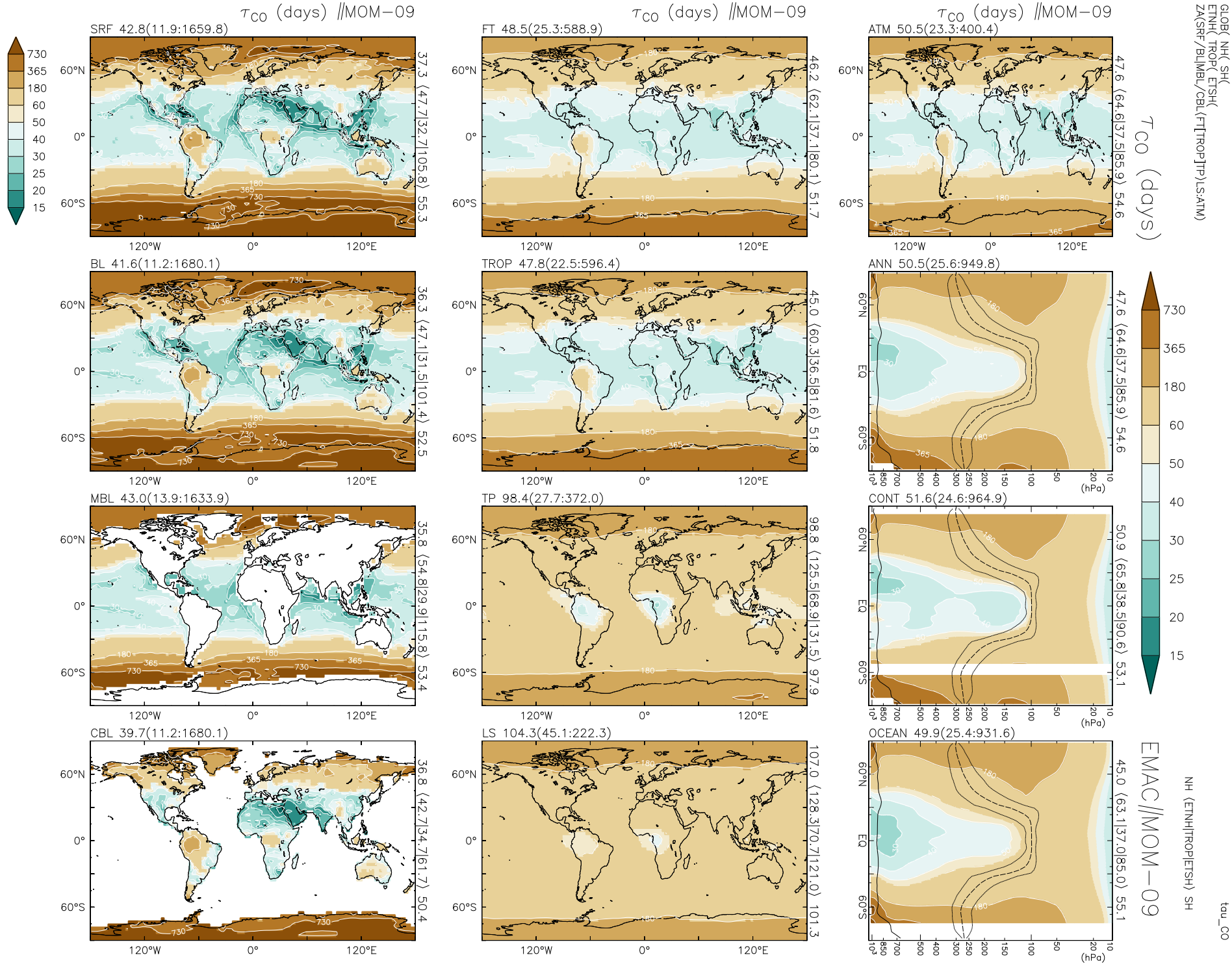
S6


OH reactivity (s$^{-1}$) //MOM-09
SRF 2.6(0.3:109.4)
FT 0.6(0.3:2.0)
ATM 0.3(0.1:0.9)
BL 2.1(0.4:98.1)
TROP 0.7(0.3:2.5)
ANN 0.3(0.0:3.6)
MBL 1.4(0.7:3.4)
TP 0.1(0.1:0.3)
CONT 0.3(0.0:9.8)
CBL 3.6(0.4:98.1)
LS 0.1(0.1:0.1)
OCEAN 0.3(0.0:1.7)
50
20
10
5
4
3
2
1
0.5
0.2
0.1
0.05
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
OH reactivity (s$^{-1}$)
EMAC //MOM-09
GLOB(2.6/2.1|1.4/3.6(0.6[0.7]0.1)0.1:0.3) NH(2.7/2.2|1.5/3.1(0.6[0.7]0.1)0.1:0.3) SH(2.6/2.1|1.3/4.9(0.6[0.6]0.1)0.1:0.3)
ETNH(2.6/2.2|1.5/2.7(0.7[0.8]0.2)0.1:0.3) TROP(2.8/2.2|1.5/4.5(0.6[0.7]0.1)0.1:0.3) ETSH(1.7/1.6|1.1/3.1(0.5[0.5]0.1)0.1:0.2)
ZA(SRF/BL|MBL/CBL(FT|TROPT|P)LS:ATM)
NH (ETNH|TROP|ETSH) SH
OH_reac

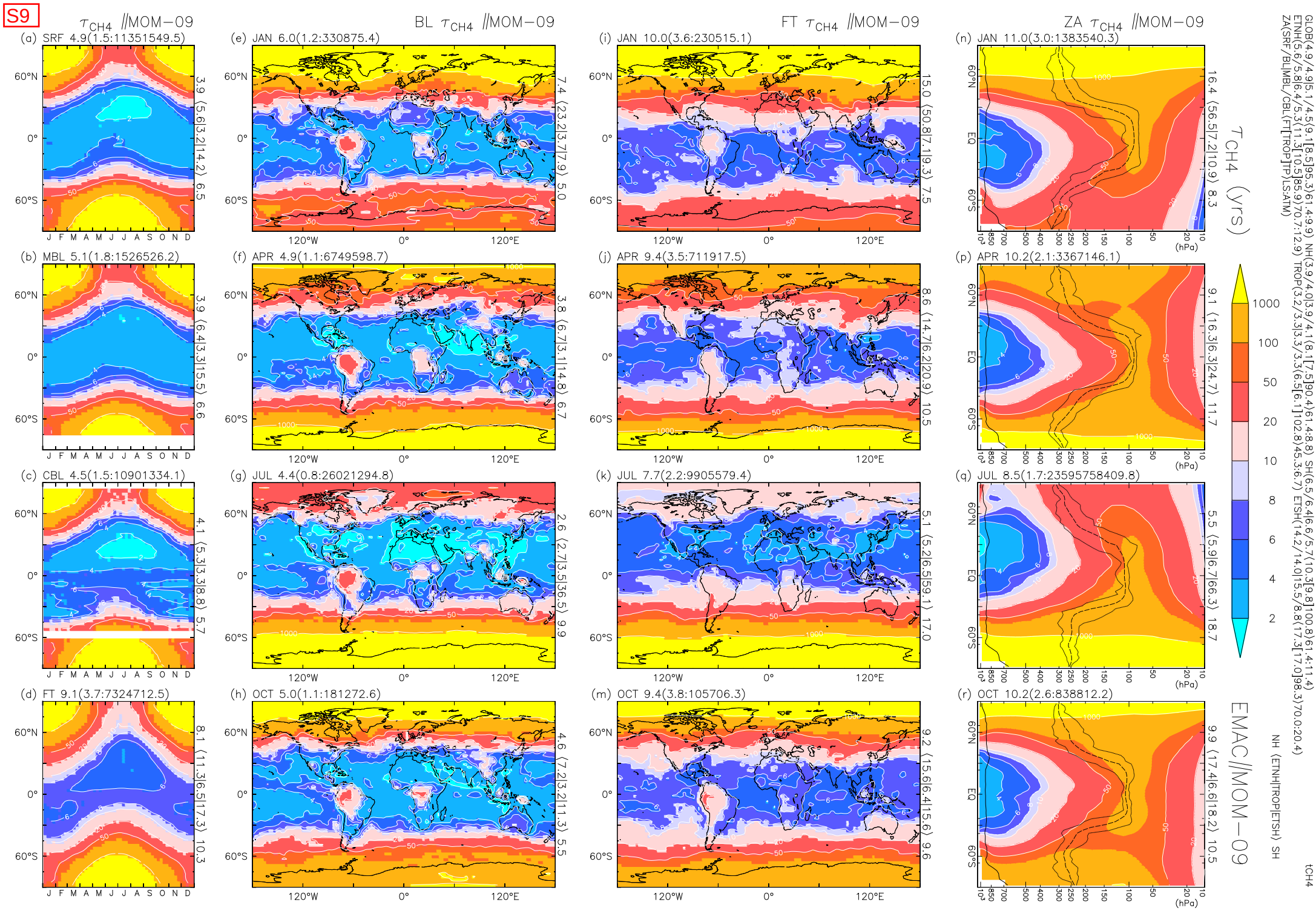
S7


τCO //MOM−09
BL τCO //MOM−09
FT τCO //MOM−09
ZA τCO //MOM−09
(a) SRF 42.8(15.3:14867932.9)
(b) MBL 43.0(15.9:4108589.2)
(c) CBL 39.7(16.0:15185286.6)
(d) FT 48.5(21.6:12158762.0)
(e) JAN 51.6(11.6:942247.3)
(f) APR 39.4(10.4:9558803.1)
(g) JUL 37.0(7.8:18791410.0)
(h) OCT 43.0(10.4:589868.3)
(i) JAN 54.7(19.5:561630.7)
(j) APR 49.0(19.5:1291998.1)
(k) JUL 41.1(14.6:12167689.9)
(m) OCT 50.0(22.5:279671.6)
(n) JAN 57.2(17.6:1927891.1)
(p) APR 50.9(21.2:3802746.3)
(q) JUL 43.2(17.0:6927088429.7)
(r) OCT 51.9(26.6:1218073.5)
J F M A M J J A S O N D
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
τCO (days)
730
365
180
60
50
40
30
25
20
15
GLOB( NH( SH(
ETNH( TROP( ETSH(
ZA(SRF/BL|MBL/CBL(FT[TROPT|TP\LS:ATM)
EMAC //MOM−09
NH ⟨ETNH|TROP|ETSH⟩ SH
tau_CO

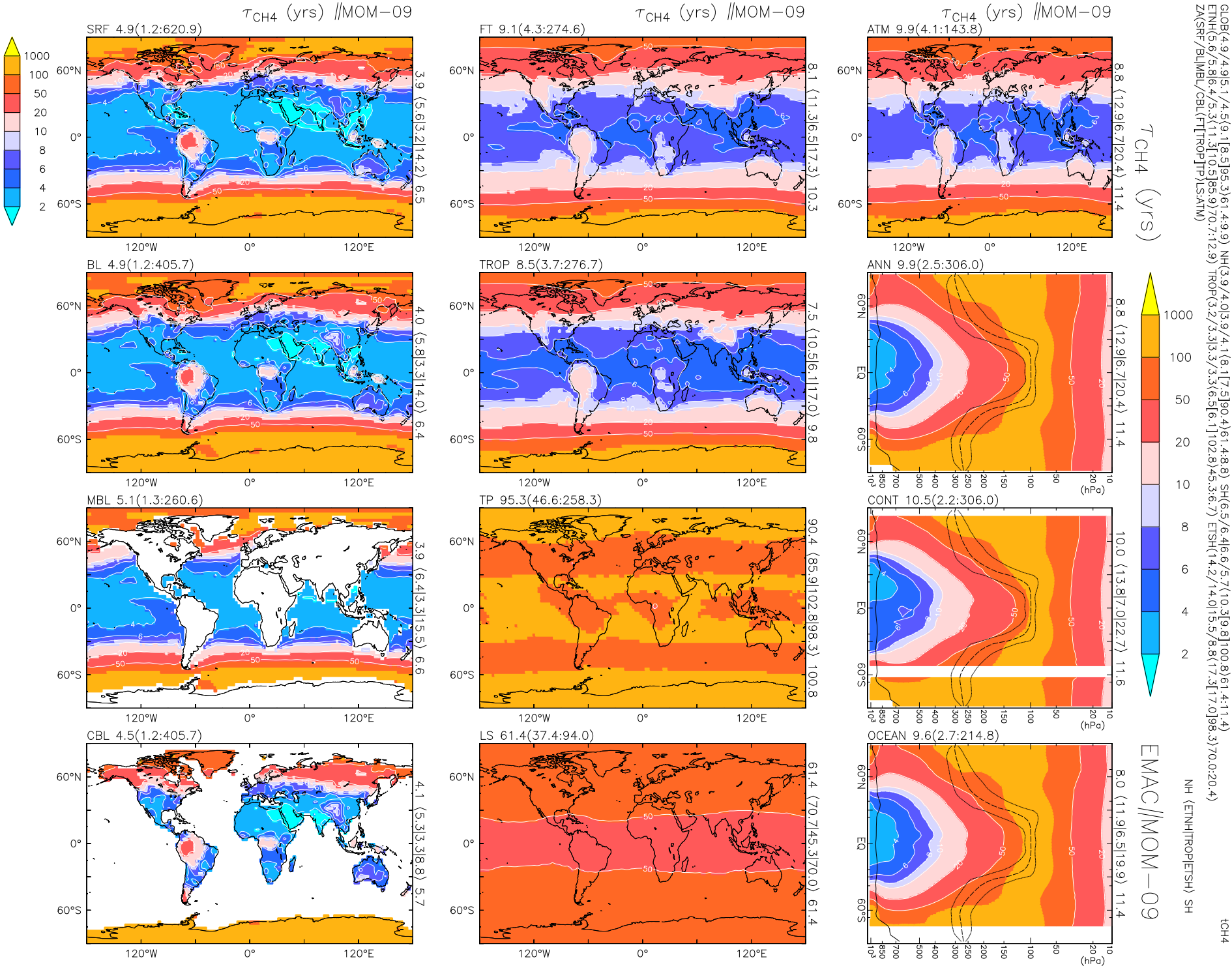
S8


τCO (days) //MOM−09
SRF 42.8(11.9:1659.8)
FT 48.5(25.3:588.9)
ATM 50.5(23.3:400.4)
BL 41.6(11.2:1680.1)
TROP 47.8(22.5:596.4)
ANN 50.5(25.6:949.8)
MBL 43.0(13.9:1633.9)
TP 98.4(27.7:372.0)
CONT 51.6(24.6:964.9)
CBL 39.7(11.2:1680.1)
LS 104.3(45.1:222.3)
OCEAN 49.9(25.4:931.6)
730
365
180
60
50
40
30
25
20
15
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
τCO (days)
EMAC //MOM−09
GLOB( NH( SH(
ETNH( TROP( ETSH(
ZA(SRF/BL/MBL/CBL(FT[TROPT]P\LS:ATM)
NH ⟨ETNH|TROP|ETSH⟩ SH
tau_CO

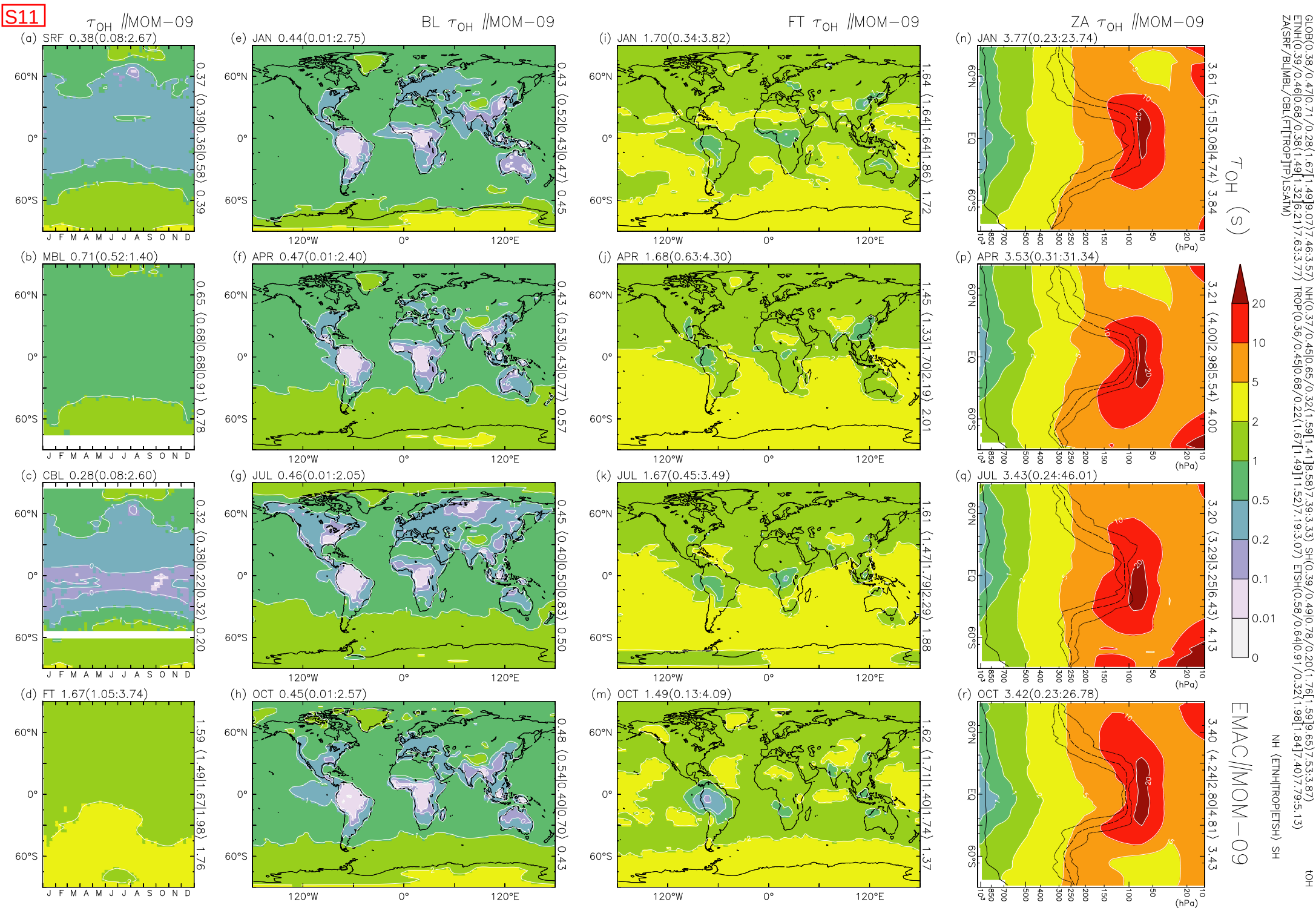
S9


τCH4 //MOM−09
BL τCH4 //MOM−09
FT τCH4 //MOM−09
ZA τCH4 //MOM−09
(a) SRF 4.9(1.5:11351549.5)
(b) MBL 5.1(1.8:1526526.2)
(c) CBL 4.5(1.5:10901334.1)
(d) FT 9.1(3.7:7324712.5)
(e) JAN 6.0(1.2:330875.4)
(f) APR 4.9(1.1:6749598.7)
(g) JUL 4.4(0.8:26021294.8)
(h) OCT 5.0(1.1:181272.6)
(i) JAN 10.0(3.6:230515.1)
(j) APR 9.4(3.5:711917.5)
(k) JUL 7.7(2.2:9905579.4)
(m) OCT 9.4(3.8:105706.3)
(n) JAN 11.0(3.0:1383540.3)
(p) APR 10.2(2.1:3367146.1)
(q) JUL 8.5(1.7:23595758409.8)
(r) OCT 10.2(2.6:838812.2)
3.9 ⟨5.6|3.2|14.2⟩ 6.5
3.9 ⟨6.4|3.3|15.5⟩ 6.6
4.1 ⟨5.3|3.3|8.8⟩ 5.7
8.1 ⟨11.3|6.5|17.3⟩ 10.3
7.4 ⟨23.2|3.7|7.9⟩ 5.0
3.8 ⟨6.7|3.1|14.8⟩ 6.7
2.6 ⟨2.7|3.5|36.5⟩ 9.9
4.6 ⟨7.2|3.2|11.3⟩ 5.5
15.0 ⟨50.8|7.1|9.3⟩ 7.5
8.6 ⟨14.7|6.2|20.9⟩ 10.5
5.1 ⟨5.2|6.5|59.1⟩ 17.0
9.2 ⟨15.6|6.4|15.6⟩ 9.6
16.4 ⟨56.5|7.2|10.9⟩ 8.3
9.1 ⟨16.3|6.3|24.7⟩ 11.7
5.5 ⟨5.9|6.7|66.3⟩ 18.7
9.9 ⟨17.4|6.6|18.2⟩ 10.5
60°N
0°
60°S
EQ
120°W
0°
120°E
J F M A M J J A S O N D
10³ 850 700 500 400 300 250 200 150 100 50 20 10 (hPa)
τCH4 (yrs)
1000
100
50
20
10
8
6
4
2
EMAC //MOM−09
NH ⟨ETNH|TROP|ETSH⟩ SH
tCH4
GLOB(4.9/4.9|5.1/4.5|9.1|8.5|95.3)61.4:9.9) NH(3.9/4.0|3.9/4.1|8.1|7.5|90.4)61.4:8.8) SH(6.5/6.4|6.6/5.7|10.3|9.8|100.8)61.4:11.4)
ETNH(5.6/5.8|6.4/5.3|11.3|10.5|85.9)70.7:12.9) TROP(3.2/3.3|3.3/3.3|6.5|6.1|102.8)45.3:6.7) ETSH(14.2/14.0|15.5/8.8(17.3|17.0|98.3)70.0:20.4)
ZA(SRF/BLMBL/CBL(FT|TROPT|P/LS:ATM)

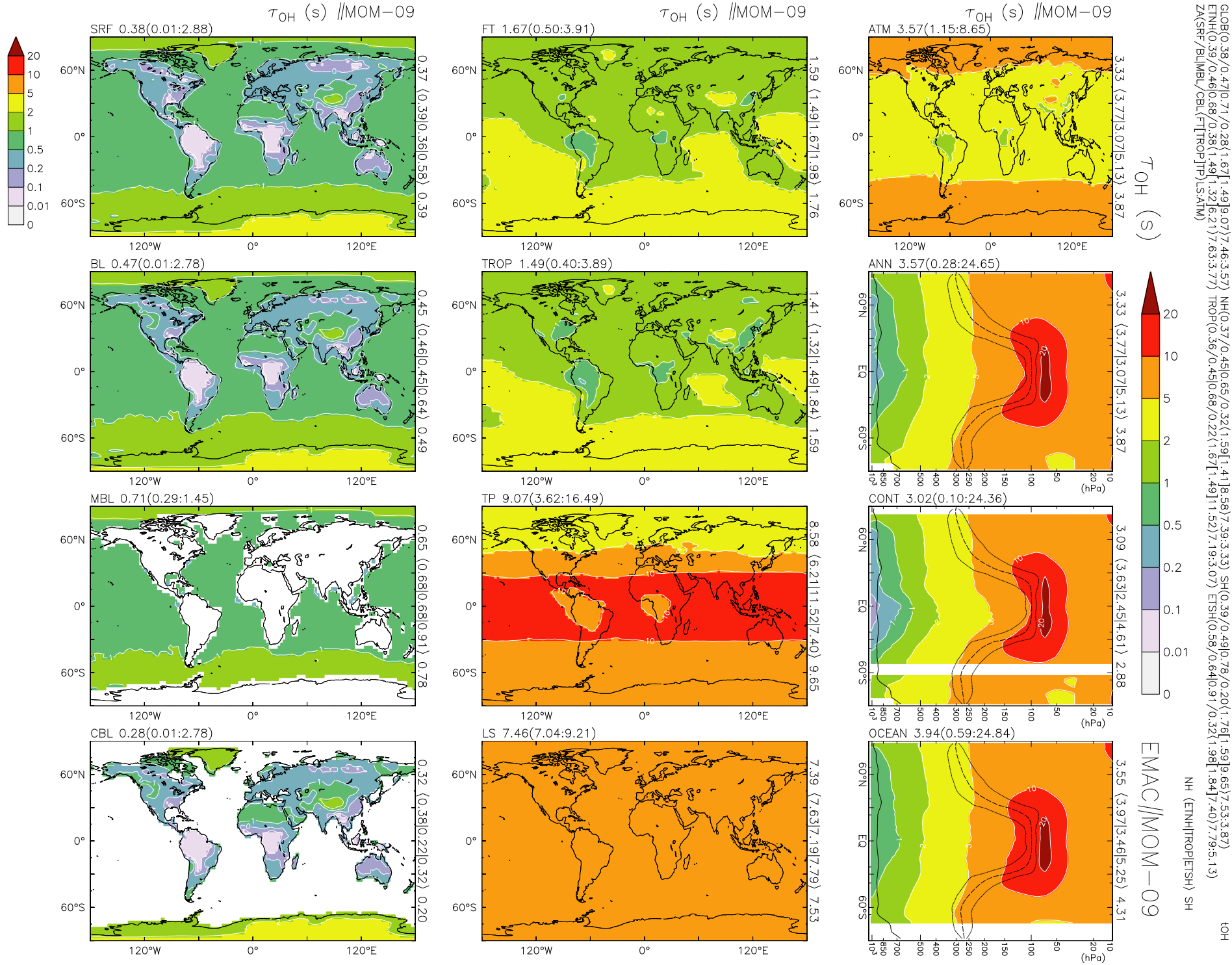
S10


τCH4 (yrs) //MOM-09
SRF 4.9(1.2:620.9)
FT 9.1(4.3:274.6)
ATM 9.9(4.1:143.8)
BL 4.9(1.2:405.7)
TROP 8.5(3.7:276.7)
ANN 9.9(2.5:306.0)
MBL 5.1(1.3:260.6)
TP 95.3(46.6:258.3)
CONT 10.5(2.2:306.0)
CBL 4.5(1.2:405.7)
LS 61.4(37.4:94.0)
OCEAN 9.6(2.7:214.8)
1000
100
50
20
10
8
6
4
2
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
3.9 (5.6|3.2|14.2) 6.5
8.1 (11.3|6.5|17.3) 10.3
8.8 (12.9|6.7|20.4) 11.4
4.0 (5.8|3.3|14.0) 6.4
7.5 (10.5|6.1|17.0) 9.8
8.8 (12.9|6.7|20.4) 11.4
3.9 (6.4|3.3|15.5) 6.6
90.4 (85.9|102.8|98.3) 100.8
10.0 (13.8|7.0|22.7) 11.6
4.1 (5.3|3.3|8.8) 5.7
61.4 (70.7|45.3|70.0) 61.4
8.0 (11.9|6.5|19.9) 11.4
τCH4 (yrs)
EMAC //MOM-09
GLOB(4.9/4.9|5.1/4.5|9.1|8.5|95.3|61.4:9.9) NH(3.9/4.0|3.9/4.1|8.1|7.5|90.4|61.4:8.8) SH(6.5/6.4|6.6/5.7|10.3|9.8|100.8|61.4:11.4)
ETNH(5.6/5.8|6.4/5.3|11.3|10.5|85.9|70.7:12.9) TROP(3.2/3.3|3.3/3.3|6.5|6.1|102.8|45.3:6.7) ETSH(14.2/14.0|15.5/8.8|17.3|17.0|98.3|70.0:20.4)
ZA(SRF/BL|MBL/CBL(FT|TROP|TP)LS:ATM)
NH (ETNH|TROP|ETSH) SH
tCH4

S11


τOH //MOM−09
BL τOH //MOM−09
FT τOH //MOM−09
ZA τOH //MOM−09
(a) SRF 0.38(0.08:2.67)
(b) MBL 0.71(0.52:1.40)
(c) CBL 0.28(0.08:2.60)
(d) FT 1.67(1.05:3.74)
(e) JAN 0.44(0.01:2.75)
(f) APR 0.47(0.01:2.40)
(g) JUL 0.46(0.01:2.05)
(h) OCT 0.45(0.01:2.57)
(i) JAN 1.70(0.34:3.82)
(j) APR 1.68(0.63:4.30)
(k) JUL 1.67(0.45:3.49)
(m) OCT 1.49(0.13:4.09)
(n) JAN 3.77(0.23:23.74)
(p) APR 3.53(0.31:31.34)
(q) JUL 3.43(0.24:46.01)
(r) OCT 3.42(0.23:26.78)
J F M A M J J A S O N D
60°N
0°
60°S
120°W
0°
120°E
EQ
(hPa)
τOH (s)
20
10
5
2
1
0.5
0.2
0.1
0.01
0
EMAC //MOM−09
GLOB⟨0.38/0.47|0.71/0.28|1.67|1.49|9.07⟩7.46:3.57) NH⟨0.37/0.45|0.65/0.32|1.59|1.41|8.58⟩7.39:3.33) SH⟨0.39/0.49|0.78/0.20|1.76|1.59|9.65⟩7.53:3.87)
ETNH⟨0.39/0.46|0.68/0.38|1.49|1.32|6.21⟩7.63:3.77) TROP⟨0.36/0.45|0.68/0.22|1.67|1.49|11.52⟩7.19:3.07) ETSH⟨0.58/0.64|0.91/0.32|1.98|1.84|7.40⟩7.79:5.13)
ZA⟨SRF/BL|MBL/CBL|FT|TROP|TP|LS:ATM⟩
NH ⟨ETNH|TROP|ETSH⟩ SH
tOH

S12

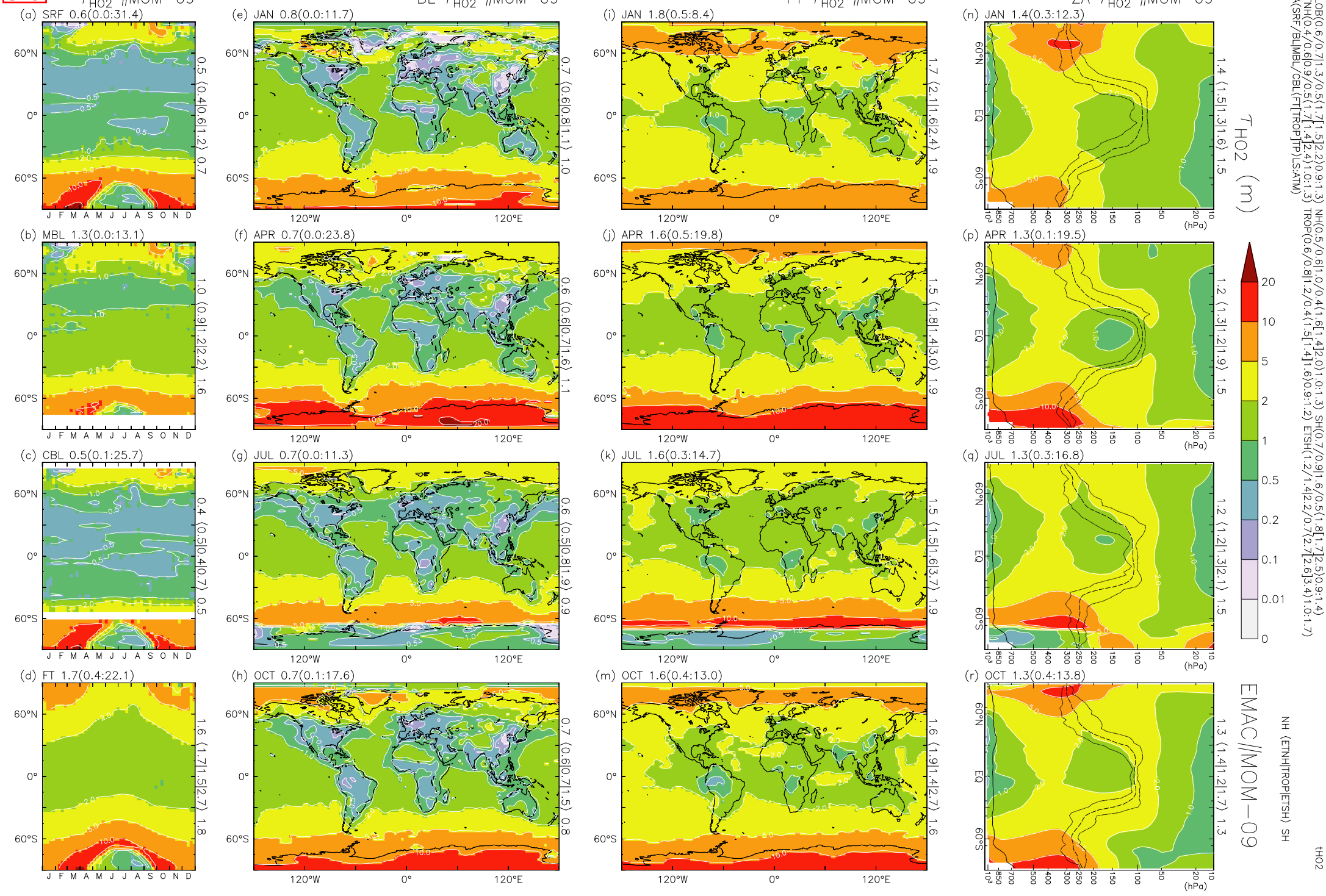



GLOB(0.38/0.47|0.71/0.28(1.67|1.49|9.07)7.46:3.57) NH(0.37/0.45|0.65/0.32(1.59|1.41|8.58)7.39:3.33) SH(0.39/0.49|0.78/0.20(1.76|1.59|9.65)7.53:3.87)
ETNH(0.39/0.46|0.68/0.38(1.49|1.32|6.21)7.63:3.77) TROP(0.36/0.45|0.68/0.22(1.67|1.49|11.52)7.19:3.07) ETSH(0.58/0.64|0.91/0.32(1.98|1.84|7.40)7.79:5.13)
ZA(SRF/BL|MBL/CBL(FT|TROPT|P)LS:ATM)

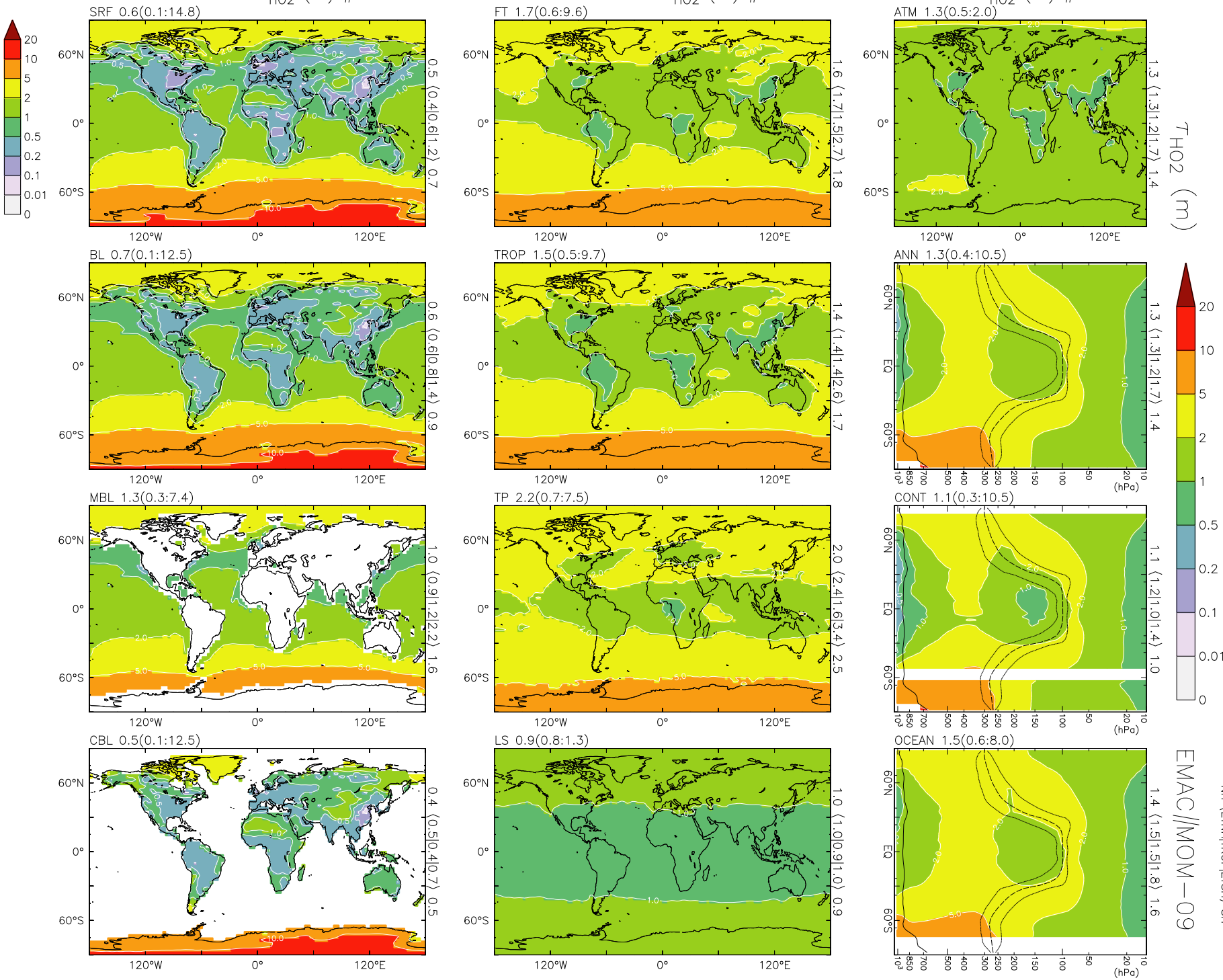
NH (ETNH|TROP|ETSH) SH

tOH

S13


τHO2 //MOM−09
BL τHO2 //MOM−09
FT τHO2 //MOM−09
ZA τHO2 //MOM−09
(a) SRF 0.6(0.0:31.4)
(b) MBL 1.3(0.0:13.1)
(c) CBL 0.5(0.1:25.7)
(d) FT 1.7(0.4:22.1)
(e) JAN 0.8(0.0:11.7)
(f) APR 0.7(0.0:23.8)
(g) JUL 0.7(0.0:11.3)
(h) OCT 0.7(0.1:17.6)
(i) JAN 1.8(0.5:8.4)
(j) APR 1.6(0.5:19.8)
(k) JUL 1.6(0.3:14.7)
(m) OCT 1.6(0.4:13.0)
(n) JAN 1.4(0.3:12.3)
(p) APR 1.3(0.1:19.5)
(q) JUL 1.3(0.3:16.8)
(r) OCT 1.3(0.4:13.8)
60°N
0°
60°S
120°W
120°E
J F M A M J J A S O N D
EQ
(hPa)
τHO2 (m)
20
10
5
2
1
0.5
0.2
0.1
0.01
0
EMAC //MOM−09
NH ⟨ETNH|TROP|ETSH⟩ SH
tHO2
GLOB(0.6/0.7|1.3/0.5(1.7|1.5]2.2)0.9:1.3) NH(0.5/0.6|1.0/0.4(1.6|1.4]2.0)1.0:1.3) SH(0.7/0.9|1.6/0.5(1.8|1.7]2.5)0.9:1.4)
ETNH(0.4/0.6|0.9/0.5(1.7|1.4]2.4)1.0:1.3) TROP(0.6/0.8|1.2/0.4(1.5|1.4]1.6)0.9:1.2) ETSH(1.2/1.4|2.2/0.7(2.7|2.6]3.4)1.0:1.7)
ZA(SRF/BL|MBL/CBL(FT|TROP]TP|LS:ATM)

S14


τHO2 (m) //MOM-09
SRF 0.6(0.1:14.8)
FT 1.7(0.6:9.6)
ATM 1.3(0.5:2.0)
BL 0.7(0.1:12.5)
TROP 1.5(0.5:9.7)
ANN 1.3(0.4:10.5)
MBL 1.3(0.3:7.4)
TP 2.2(0.7:7.5)
CONT 1.1(0.3:10.5)
CBL 0.5(0.1:12.5)
LS 0.9(0.8:1.3)
OCEAN 1.5(0.6:8.0)
τHO2 (m)
EMAC//MOM-09
NH (ETNH|TROP|ETSH) SH
tHO2
GLOB(0.6/0.7|1.3/0.5(1.7|1.5|2.2)0.9:1.3) NH(0.5/0.6|1.0/0.4(1.6|1.4|2.0)1.0:1.3) SH(0.7/0.9|1.6/0.5(1.8|1.7|2.5)0.9:1.4)
ETNH(0.4/0.6|0.9/0.5(1.7|1.4|2.4)1.0:1.3) TROP(0.6/0.8|1.2/0.4(1.5|1.4|1.6)0.9:1.2) ETSH(1.2/1.4|2.2/0.7(2.7|2.6|3.4)1.0:1.7)
ZA(SRF/BL|MBL/CBL(FT|TROP|TP)LS:ATM)

S15

## EMAC/MOM simulated annual OH concentrations by domain [$10^5$ molecules $cm^{-3}$]

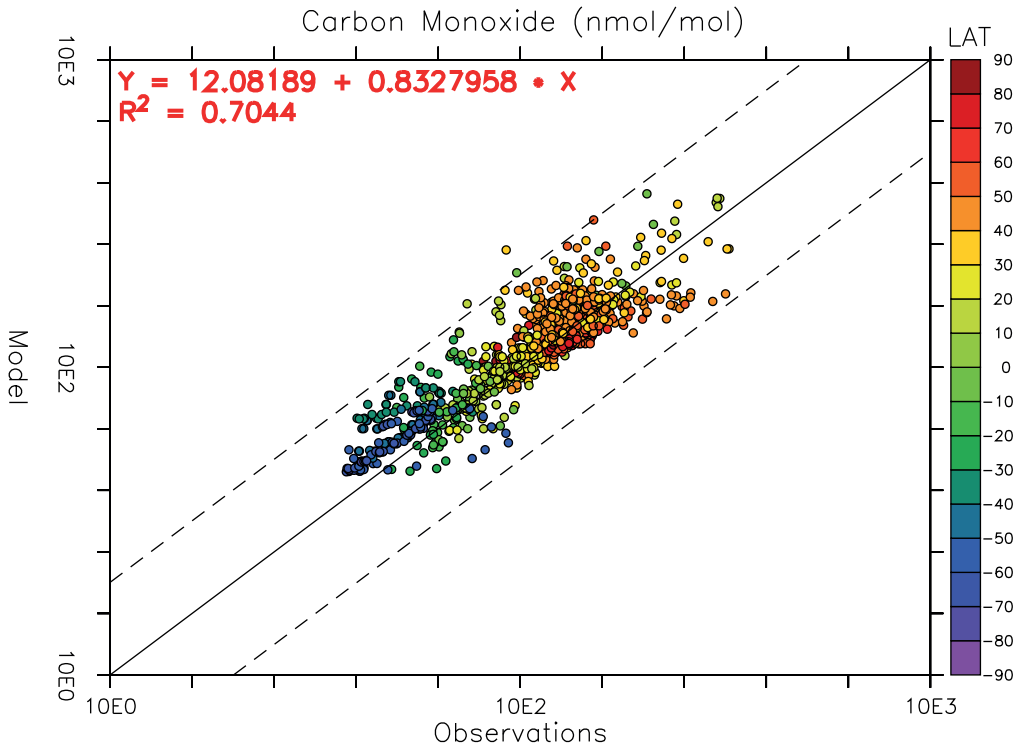
| domain / vertical | GLOB | ETNH | IT | ETSH | NH | SH | iNH | iSH | ARC | ANT | NH/SH rel.ratio EQ metric | NH/SH rel.ratio ITCZ metric |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | EQ metric | | ITCZ metric | | >66°N | >60°S | | |
| **air volume-weighted** | | | | | | | | | | | | |
| SRF | 10.9 | 10.4 | 15.3 | 4.2 | 13.5 | 7.9 | 13.5 | 8.5 | 1.3 | 0.6 | +70% | +59% |
| BL | 11.3 | 10.8 | 15.8 | 4.6 | 13.9 | 8.6 | 14.0 | 9.1 | 1.2 | 0.7 | +63% | +54% |
| MBL | 10.8 | 9.5 | 16.1 | 4.1 | 13.9 | 8.3 | 14.1 | 8.9 | 0.9 | 0.6 | +68% | +59% |
| CBL | 12.5 | 11.8 | 14.8 | 7.1 | 13.9 | 9.8 | 13.8 | 10.0 | 1.5 | 0.8 | +42% | +37% |
| FT | 11.3 | 9.1 | 14.6 | 6.7 | 12.0 | 10.2 | 12.0 | 10.7 | 3.3 | 1.7 | +18% | +12% |
| T | 11.3 | 9.2 | 14.6 | 6.6 | 12.1 | 10.1 | 12.1 | 10.6 | 3.2 | 1.7 | +20% | +13% |
| TP | 7.1 | 5.6 | 9.2 | 5.0 | 7.0 | 6.6 | 7.2 | 7.0 | 3.1 | 2.4 | +6% | +3% |
| LS | 14.6 | 12.8 | 17.5 | 12.8 | 14.5 | 14.4 | 14.4 | 14.7 | 9.4 | 10.1 | +1% | −2% |
| ATM | 13.5 | 11.8 | 16.4 | 11.1 | 13.7 | 13.0 | 13.7 | 13.4 | 8.1 | 8.3 | +5% | +2% |
| **air mass-weighted** | | | | | | | | | | | | |
| SRF | 10.6 | 10.0 | 15.3 | 4.2 | 13.2 | 7.8 | 13.2 | 8.3 | 1.2 | 0.6 | +69% | +58% |
| BL | 11.1 | 10.3 | 15.8 | 4.4 | 13.6 | 8.4 | 13.6 | 8.9 | 1.2 | 0.7 | +62% | +53% |
| MBL | 10.6 | 9.3 | 16.1 | 4.1 | 13.7 | 8.1 | 13.9 | 8.7 | 0.9 | 0.6 | +69% | +60% |
| CBL | 12.1 | 11.1 | 14.8 | 6.9 | 13.4 | 9.7 | 13.2 | 9.9 | 1.5 | 0.8 | +38% | +34% |
| FT | 11.1 | 9.0 | 15.0 | 6.5 | 12.0 | 9.8 | 11.9 | 10.4 | 3.1 | 1.6 | +22% | +15% |
| T | 11.1 | 9.1 | 15.1 | 6.3 | 12.1 | 9.7 | 12.0 | 10.3 | 3.0 | 1.6 | +25% | +17% |
| TP | 6.4 | 5.2 | 9.5 | 4.7 | 6.5 | 6.0 | 6.6 | 6.3 | 2.9 | 2.5 | +8% | +4% |
| LS | 7.0 | 5.8 | 10.6 | 5.8 | 6.9 | 6.9 | 6.9 | 7.1 | 3.9 | 4.0 | +1% | −3% |
| ATM | 10.3 | 8.3 | 14.6 | 6.2 | 11.1 | 9.1 | 11.1 | 9.7 | 3.3 | 2.4 | +22% | +14% |
| **$CH_4$ sink-weighted** | | | | | | | | | | | | |
| SRF | 12.2 | 12.2 | 15.4 | 5.0 | 15.0 | 9.0 | 15.0 | 9.6 | 1.5 | 0.7 | +66% | +57% |
| BL | 12.5 | 12.2 | 15.9 | 5.2 | 15.2 | 9.5 | 15.2 | 10.0 | 1.5 | 0.7 | +60% | +52% |
| MBL | 11.8 | 10.7 | 16.2 | 4.6 | 14.8 | 9.2 | 15.0 | 9.8 | 1.1 | 0.7 | +61% | +53% |
| CBL | 14.0 | 13.7 | 15.0 | 9.0 | 15.7 | 10.9 | 15.5 | 11.1 | 1.8 | 0.9 | +44% | +40% |
| FT | 12.4 | 10.8 | 15.6 | 7.4 | 13.6 | 10.9 | 13.5 | 11.5 | 3.8 | 1.7 | +25% | +18% |
| T | 12.4 | 11.0 | 15.6 | 7.1 | 13.8 | 10.7 | 13.8 | 11.2 | 3.6 | 1.6 | +30% | +22% |
| TP | 5.9 | 5.4 | 9.4 | 4.8 | 6.1 | 5.5 | 6.1 | 5.8 | 3.4 | 3.0 | +10% | +6% |
| LS | 7.7 | 6.2 | 12.7 | 6.4 | 7.4 | 7.6 | 7.4 | 7.9 | 4.5 | 5.3 | −2% | −6% |
| ATM | 12.2 | 10.7 | 15.6 | 7.0 | 13.5 | 10.5 | 13.5 | 11.1 | 3.7 | 2.2 | +29% | +21% |
| **MCF sink-weighted** | | | | | | | | | | | | |
| SRF | 12.0 | 11.6 | 15.4 | 5.0 | 14.5 | 9.0 | 14.5 | 9.5 | 1.5 | 0.7 | +62% | +53% |
| BL | 12.3 | 11.7 | 15.9 | 5.2 | 14.8 | 9.4 | 14.8 | 9.9 | 1.5 | 0.8 | +56% | +49% |
| MBL | 11.7 | 10.2 | 16.2 | 4.6 | 14.5 | 9.1 | 14.7 | 9.7 | 1.1 | 0.7 | +58% | +52% |
| CBL | 13.7 | 13.1 | 15.0 | 8.9 | 15.2 | 10.9 | 14.9 | 11.0 | 1.9 | 0.9 | +40% | +35% |
| FT | 12.3 | 10.4 | 15.5 | 7.5 | 13.2 | 10.9 | 13.1 | 11.4 | 3.9 | 1.8 | +21% | +15% |
| T | 12.3 | 10.6 | 15.6 | 7.2 | 13.4 | 10.7 | 13.3 | 11.2 | 3.7 | 1.7 | +25% | +19% |
| TP | 5.9 | 5.3 | 9.4 | 4.9 | 6.0 | 5.6 | 6.0 | 5.8 | 3.4 | 3.0 | +6% | +3% |
| LS | 4.9 | 4.4 | 7.5 | 4.5 | 4.8 | 4.9 | 4.8 | 5.0 | 3.4 | 3.7 | −2% | −4% |
| ATM | 12.0 | 10.2 | 15.5 | 7.0 | 13.0 | 10.5 | 13.0 | 11.0 | 3.6 | 2.0 | +25% | +18% |

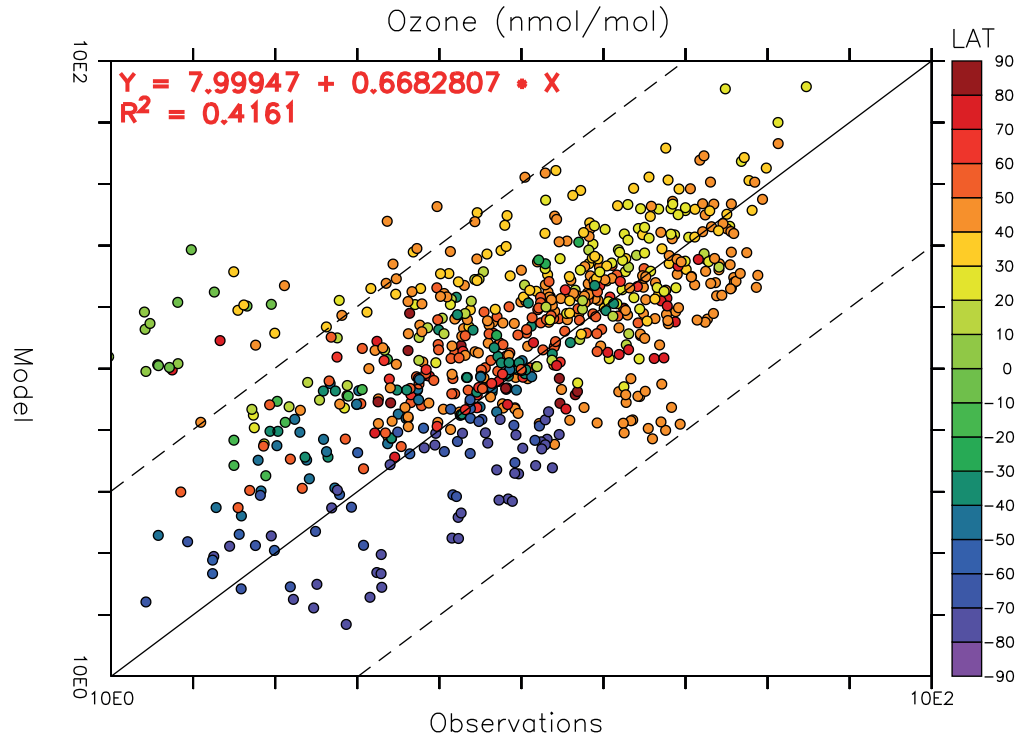
Abbreviations:

| | | | | | |
|---|---|---|---|---|---|
| zonal: | GLOB | global (90°S–90°N) | NH/SH | Northern/Southern Hemisphere | |
| | IT/ET | intra/extra-tropics (separated at 24.6°N/S) | iSH/iNH | ITCZ-separated NH/SH | |
| | EQ/ITCZ | Equator/Intertropical Convergence Zone | ARC/ANT | Arctic (>66°N)/Antarctic (>60°S) | |
| vertical: | SRF/TP | surface/tropopause | T | troposphere (below the TP) | |
| | (M/C)BL | (marine/continental) boundary layer | FT | free troposphere (above the BL, below the TP) | |
| | LS | lower stratosphere (above the TP) | ATM | entire model domain | |

S16

Monthly mean surface mixing ratios (nmol/mol) from the WDCGG World Data Center at http://ds.data.jma.go.jp/gmd/wdcgg/ and EMAC for the year 2013 (latitude color coded)



## Prescribed and on-line calculated direct emission fluxes in EMAC/MOM

| | Compound | Emission Category | | | Units |
|---|---|---|---|---|---|
| | | Anthopogenic [a] | Biogenic [b] | Biomass Burning [c] | |
| $C_1$ | Formic Acid | 2.12 | 0.80 – 0.82 | 0.62 – 0.80 | TgC/yr |
| | Hydrogen Cyanide | | 0.28 – 0.29 | 0.91 – 1.39 | |
| | Formaldehyde | 1.37 | 1.83 – 1.90 | 1.53 – 1.99 | |
| | Carbon Monoxide | 251.0 | 40.5 – 41.9 | 111.6 – 149.5 | |
| | Methanol | 1.67 | 34.7 – 36.0 | 2.17 – 2.95 | |
| | Methylnitrate | | | 0.01 – 0.03 | |
| $C_2$ | Glycolaldehyde | | | 1.62 – 2.10 | |
| | Acetic Acid | 4.24 | 1.22 – 1.26 | 4.85 – 6.40 | |
| | Acetonitrile | | | 0.55 – 0.91 | |
| | Acetaldehyde | 2.73 | 6.99 – 7.40 | 1.24 – 1.59 | |
| | Ethane | 2.67 | 0.25 – 0.26 | 2.23 – 2.84 | |
| | Ethyl Alcohol | | 6.68 – 7.07 | | |
| | Ethene | 6.50 | 17.51 – 18.1 | 2.80 – 3.69 | |
| | Ethyne | 2.96 | | 0.83 – 1.04 | |
| $C_3$ | Pyruvic Acid | | 0.13 – 0.13 | | |
| | Acetone | 1.69 | 19.4 – 20.2 | 0.73 – 1.00 | |
| | Propane | 3.27 | 0.13 – 0.13 | 0.43 – 0.56 | |
| | Propene | 2.97 | 10.8 – 11.2 | 2.37 – 3.19 | |
| | Propanal | | | 0.04 – 0.04 | |
| | Hydroxy Acetone | | | 0.96 – 1.28 | |
| $C_4$ | Trans-2-Butene | 4.03 | | 0.06 – 0.07 | |
| | N-Butane | 8.31 | | 0.10 – 0.13 | |
| | Methyl Vinyl Ketone | | | 0.24 – 0.29 | |
| | 2-Methylpropene | 4.03 | | 0.16 – 0.20 | |
| | Methyl Ethyl Ketone | 2.25 | 0.10 – 0.11 | 0.21 – 0.26 | |
| | Methacrolein | | | 0.14 – 0.17 | |
| | Methylpropanal | | | 0.07 – 0.09 | |
| | Iso-Butane | 8.31 | | 0.03 – 0.04 | |
| | Cis-2-Butene | 4.03 | | 0.04 – 0.06 | |
| | 1-Butene | 4.03 | 4.71 – 4.88 | 0.20 – 0.25 | |
| | Biacetyl | | | 0.25 – 0.29 | |
| $C_5$ | Methylbutenol | | 0.80 – 0.86 | | |
| | Isoprene | | 545.5 – 578.3 | 0.27 – 0.43 | |
| $C_6$ | Phenol | 2.62 | | 1.31 – 1.96 | |
| | Benzene | 6.27 | | 1.26 – 1.73 | |
| $C_7$ | Toluene | 6.99 | 0.29 – 0.30 | 0.70 – 1.12 | |
| | Benzaldehyde | 3.05 | 0.02 – 0.03 | 0.08 – 0.10 | |
| $C_8$ | Styrene | 3.49 | | 0.15 – 0.20 | |
| | Xylene | 6.05 | | 0.23 – 0.30 | |
| | Ethylbenzene | 3.49 | | 0.52 – 0.67 | |
| $C_9$ | Trimethylbenzenes | 1.36 | | 0.07 – 0.09 | |
| $C_{10}$ | Sabinene | | 5.58 – 5.78 | | |
| | Carene | | 5.47 – 5.72 | | |
| | Camphene | | 2.52 – 2.61 | | |
| | Beta Pinene | | 14.7 – 15.3 | | |
| | Alpha Pinene | | 26.0 – 27.0 | | |
| $C_{11+}$ | Higher Aromatics | 4.80 | | | |
| | Total C: | 356.3 | 746.7 – 787.5 | 141.6 – 189.7 | |
| | Total NMVOCs: | 105.3 | 706.2 – 745.6 | 20.6 – 26.9 | |
| | | | Grand total: | 1244.6 – 1333.5 | |
| | Nitric Oxide | 33.1 | (5.0 – 5.2)* | 3.7 – 4.7 | TgN/yr |
| | Ammonia | 34.7 | | 3.1 – 5.5 | |
| | Nitrous Acid | | | 0.43 – 0.54 | |
| | Total N: | 67.7 | | 7.4 – 11.0 | |
| | | | Grand total: | 80.1 – 83.9 | |
| | Sulfur Dioxide | 41.6 | | 0.89 – 1.17 | TgS/yr |
| | | | Grand total: | 42.53 – 42.81 | |

Notes: Ranges represent interannual variation

[a] RCP8.5 scenario (Riahi et al., 2007; Yoon and Pozzer, 2014)

[b] MEGAN submodel (Guenther et al., 2012)

[c] BIOBURN submodel (Carbrera-Perez et al., 2016)

* Lightning $NO_X$ source (LNOX submodel, Grewe et al., 2001)


**References:**

Cabrera-Perez, D., Taraborrelli, D., Sander, R., and Pozzer, A.: Global atmospheric budget of simple monocyclic aromatic compounds, *Atmos. Chem. Phys. Discuss.*, 16, 1–25, 2016.

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{This file was created automatically by xmecca, DO NOT EDIT!}
{xmecca was run on 2015-11-14 at 19:50:16 by sgromov on machine hydra05}
{***** START: gas-phase species from gas_mom.spc *****}

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

#INCLUDE atoms
Min; {minus (negative charge as pseudo-atom for charge balance)}
Pls; {plus  (positive charge as pseudo-atom for charge balance)}
{end of atom definitions}

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

{ 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}
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}             {}
NH2OH           = 2H +  O +  N      ; {@NH2OH}           {}
NH2O            = 2H +  O +  N      ; {@NH_2O}           {}
NH2OH           = 3H +  O +  N      ; {@NH_2OH}          {}
LNITROGEN       =           N       ; {@LNITROGEN}       {lumped N species}

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

{1C}
CO              =  C       +  O     ; {@CO}              {carbon monoxide}
CO2             =  C       + 2O     ; {@CO_2}            {carbon dioxide}
HCHO            =  C + 2H  +  O     ; {@HCHO}            {methanal (formaldehyde)}
HCOOH           =  C + 2H  + 2O     ; {@HCOOH}           {formic acid}
CH2OO           =  C + 2H  + 2O     ; {@CH_2OO}          {carbonyl oxide - stabilized Criegee
Intermediate}
CH2OOA          =  C + 2H  + 2O     ; {@CH_2OO^*}        {carbonyl oxide - excited Criegee
Intermediate}
CH3             =  C + 3H           ; {@CH_3}            {methyl radical}
CH3O            =  C + 3H +  O      ; {@CH_3O}           {methoxy radical}
CH3O2           =  C + 3H + 2O      ; {@CH_3O_2}         {methylperoxy radical}
HOCH2O2         =  C + 3H + 3O      ; {@HOCH_2O_2}       {hydroxy methyl peroxy radical}
CH4             =  C + 4H           ; {@CH_4}            {methane}
CH3OH           =  C + 4H +  O      ; {@CH_3OH}          {methanol}
CH3OOH          =  C + 4H + 2O      ; {@CH_3OOH}         {methyl peroxide}
HOCH2OOH        =  C + 4H + 3O      ; {@HOCH_2OOH}       {hydroxy methyl hydroperoxide}
HOCH2OH         =  C + 4H + 2O      ; {@HOCH_2OH}        {dyhydroxy methane}
{1C (CHON)}
CH3ONO          =  C + 3H + 2O + N  ; {@CH_3ONO}         {methylnitrite}
CH3NO3          =  C + 3H + 3O + N  ; {@CH_3NO_2}        {methylnitrate}
CH3O2NO2        =  C + 3H + 4O + N  ; {@CH_3O_2NO_2}     {peroxy methylnitrate}
HOCH2O2NO2      =  C + 3H + 5O + N  ; {@HOCH_2O_2NO_2}   {hydroxy methyl peroxy nitrate}
HCN             =  C + H      + N   ; {@HCN}             {}
CN              =  C          + N   ; {@CN}              {}
NCO             =  C       +  O + N ; {@NCO}             {}
{1C (lumped)}
LCARBON         =  C                ; {@LCARBON}         {lumped C1 species}
{2C (CHO)}
HCOCO3          = 2C +  H  + 4O     ; {@HCOCO_3}         {MCM}
HCOCO           = 2C +  H  + 2O     ; {@HCOCO}           {MOM}
C2H2            = 2C + 2H           ; {@C_2H_2}          {MCM: ethyne}
CH2CO           = 2C + 2H +  O      ; {@CH2CO}           {CH2CO, ketene}
GLYOX           = 2C + 2H + 2O      ; {@GLYOX}           {MCM: CHOCHO = glyoxal}
HCOCO2H         = 2C + 2H + 3O      ; {@HCOCO_2H}        {MCM: oxoethanoic acid}
HCOCO3H         = 2C + 2H + 4O      ; {@HCOCO_3H}        {MCM}
CH3CO           = 2C + 3H + 2O      ; {@CH_3C(O)}        {MCM: acetyl radical}
HOCH2CO         = 2C + 3H + 2O      ; {@HOCH2CO}         {HOCH2CO}
HOCHCHO         = 2C + 3H + 2O      ; {@HOCHCHO}         {HOCHCHO}
HCOCH2O2        = 2C + 3H + 3O      ; {@HCOCH_2O_2}      {MCM: HCOCH2O2}
CH3CO3          = 2C + 3H + 3O      ; {@CH_3C(O)OO}      {MCM: peroxy acetyl radical}
HOCH2CO3        = 2C + 3H + 4O      ; {@HOCH_2CO_3}      {MCM}
HOOCH2CO3       = 2C + 3H + 5O      ; {@HOOCH_2CO_3}     {MIM3}
C2H4            = 2C + 4H           ; {@C_2H_4}          {MCM: ethene}
CH2CHOH         = 2C + 4H +  O      ; {@CH_2CHOH}        {vinyl alcohol}
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CH3CHO          =  2C +  4H +   0      ; {@CH_3CHO}          {MCM: acetaldehyde}
CH3CO2H         =  2C +  4H +  20      ; {@CH_3CO0H}         {MCM: acetic acid}
HOCH2CHO        =  2C +  4H +  20      ; {@HOCH_2CHO}        {MCM: glycolaldehyde}
HOOCH2CHO       =  2C +  4H +  30      ; {@HOOCH2CHO}        {HOOCH2CHO}
CH3CO3H         =  2C +  4H +  30      ; {@CH_3C(O)OOH}      {MCM: peroxy acetic acid}
HOCH2CO2H       =  2C +  4H +  30      ; {@HOCH_2CO_2H}      {MCM: hydroxyethanoic acid}
HOCH2CO3H       =  2C +  4H +  40      ; {@HOCH_2CO_3H}      {MCM}
HOOCH2CO2H      =  2C +  4H +  40      ; {@HOOCH2CO2H}       {HOOCH2CO2H}
HOOCH2CO3H      =  2C +  4H +  50      ; {@HOOCH2CO3H}       {HOOCH2CO3H}
C2H5O2          =  2C +  5H +  20      ; {@C_2H_5O_2}        {MCM: ethylperoxy radical}
HOCH2CH2O       =  2C +  5H +  20      ; {@HOCH_2CH_2O}      {MCM}
HOCH2CH2O2      =  2C +  5H +  30      ; {@HOCH_2CH_2O_2}    {MCM}
CH3CH(OH)O2     =  2C +  5H +  30      ; {@CH3CH(OH)O2}      {CH3CH(OH)O2}
C2H6            =  2C +  6H            ; {@C_2H_6}           {MCM: ethane}
C2H5OH          =  2C +  6H +   0      ; {@C_2H_5OH}         {MCM: ethyl alcohol}
C2H5OOH         =  2C +  6H +  20      ; {@C_2H_5OOH}        {MCM: ethyl hydro peroxide}
ETHGLY          =  2C +  6H +  20      ; {@ETHGLY}           {MCM: HOCH2CH2OH}
HYETHO2H        =  2C +  6H +  30      ; {@HYETHO2H}         {MCM: HOCH2CH2OOH}
CH3CH(OH)OOH    =  2C +  6H +  30      ; {@CH3CH(OH)OOH}     {CH3CH(OH)OOH}
{2C (CHON)}
NCCH2O2         =  2C +  2H +  2O +  N ; {@NCCH_2O_2}        {}
NO3CH2CO3       =  2C +  2H +  6O +  N ; {@NO_3CH2CO_3}      {MCM: NO3CH2CO3}
NO3CH2PAN       =  2C +  2H +  8O + 2N ; {@NO_3CH2CHO}       {MCM: NO3CH2PAN}
CH3CN           =  2C +  3H        + N ; {@CH_3CN}           {}
NO3CH2CHO       =  2C +  3H +  4O +  N ; {@NO_3CH2CHO}       {MCM: NO3CH2CHO}
PAN             =  2C +  3H +  5O +  N ; {@PAN}              {MCM: CH3C(O)OONO2 =
peroxyacetylnitrate}
PHAN            =  2C +  3H +  6O +  N ; {@PHAN}             {MCM: HOCH2C(O)OONO2}
ETHOHNO3        =  2C +  5H +  4O +  N ; {@ETHOHNO3}         {MCM: HOCH2CH2ONO2}
C2H5NO3         =  2C +  5H +  3O +  N ; {@C_2H_5ONO_2}      {ethyl nitrate}
C2H5O2NO2       =  2C +  5H +  4O +  N ; {@C_2H_5O_2NO_2}    {ethyl peroxy nitrate}
{3C (CHO)}
C33CO           =  3C +  2H +  3O      ; {@HCOCOCHO}         {MCM}
CH3OCH2O2       =  3C +  3H +  4O      ; {@HCOCOCH_2O_2}     {MCM}
HCOCH2CO3       =  3C +  3H +  5O      ; {@HCOCH2CO3}        {MCM: HCOCH2CO3}
ALCOCH2OOH      =  3C +  4H +  4O      ; {@HCOCOCH_2OOH}     {MCM}
MGLYOX          =  3C +  4H +  2O      ; {@MGLYOX}           {MCM: CH3COCHO = methylglyoxal}
HOCH2COCHO      =  3C +  4H +  3O      ; {@HOCH2COCHO}       {MCM}
HCOCH2CHO       =  3C +  4H +  3O      ; {@HCOCH2CHO}        {MCM: HCOCH2CHO}
HCOCH2CO2H      =  3C +  4H +  4O      ; {@HCOCH2CO2H}       {MCM: HCOCH2CO2H}
HCOCH2CO3H      =  3C +  4H +  5O      ; {@HCOCH2CO3H}       {MCM: HCOCH2CO3H}
CH3COCH2O2      =  3C +  5H +  3O      ; {@CH_3COCH_2O_2}    {MCM: peroxyradical from acetone}
HOC2H4CO3       =  3C +  5H +  4O      ; {@HOC_2H_4CO_3}     {MCM: HOC2H4CO3}
C3H6            =  3C +  6H            ; {@C_3H_6}           {MCM: propene}
CH3COCH3        =  3C +  6H +   0      ; {@CH_3COCH_3}       {MCM: acetone}
ACETOL          =  3C +  6H +  2O      ; {@CH_3COCH_2OH}     {MCM: HO-CH2-CO-CH3 = hydroxy acetone}
HYPERACET       =  3C +  6H +  3O      ; {@CH_3COCH_2O_2H}   {MCM: hydroperoxide from CH3COCH2O2}
HOC2H4CO2H      =  3C +  6H +  3O      ; {@HOC2H4CO2H}       {MCM: HOC2H4CO2H}
HOC2H4CO3H      =  3C +  6H +  4O      ; {@HOC2H4CO3H}       {MCM: HOC2H4CO3H}
IC3H7O2         =  3C +  7H +  2O      ; {@iC_3H_7O_2}       {MCM: isopropylperoxy radical}
HYPROPO2        =  3C +  7H +  3O      ; {@HYPROPO2}         {MCM: CH3CH(O2)CH2OH}
C3H8            =  3C +  8H            ; {@C_3H_8}           {MCM: propane}
IC3H7OOH        =  3C +  8H +  2O      ; {@iC_3H_7OOH}       {MCM: isopropyl hydro peroxide}
HYPROPO2H       =  3C +  8H +  3O      ; {@HYPROPO2H}        {MCM: CH3CH(OOH)CH2OH}
CH3COCO3        =  3C +  3H +  4O      ; {@CH_3COCO_3}       {CH3COCO3H}
CH3CHCO         =  3C +  4H +   O      ; {@CH3CHCO}          {CH3CHCO}
CH3COCO2H       =  3C +  4H +  3O      ; {@CH_3COCO_2H}      {CH3COCO2H, pyruvic acid}
CH3COCO3H       =  3C +  4H +  4O      ; {@CH_3COCO_3H}      {CH3COCO3H}
HCOCOCH2OOH     =  3C +  4H +  4O      ; {@HCOCOCH_2OOH}     {HCOCOCH2OOH}
C2H5CO3         =  3C +  5H +  3O      ; {@C_2H_5CO_3}       {MCM: CH_3CH_2CO_3}
HOCH2COCH2O2    =  3C +  5H +  4O      ; {@HOCH2COCH2O2}     {HOCH2COCH2O2}

C2H5CHO         =  3C +  6H +   0      ; {@C_2H_5CHO}        {MCM: propanal}
PROPENOL        =  3C +  6H +   0      ; {@CH_2CHCH_2OH}     {propenol}
C2H5CO2H        =  3C +  6H +  2O      ; {@C_2H_5CO_2H}      {MCM: CH_3CH_2CO_2H}
C2H5CO3H        =  3C +  6H +  3O      ; {@C_2H_5CO_3H}      {MCM: CH_3CH_2CO_3H}
HOCH2COCH2OOH   =  3C +  6H +  4O      ; {@HOCH2COCH2OOH}    {HOCH2COCH2OOH}
NC3H7O2         =  3C +  7H +  2O      ; {@C_3H_7O_2}        {MCM: propylperoxy radical}
IPROPOL         =  3C +  8H +   0      ; {@IPROPOL}          {MCM: isopropylic alcohol}
NPROPOL         =  3C +  8H +   0      ; {@NPROPOL}          {MCM: n-propylic alcohol}
NC3H7OOH        =  3C +  8H +  2O      ; {@C_3H_7OOH}        {MCM: propyl hydro peroxide}
{3C (CHO) aromatics}
C3DIALOOH       =  3C +  4H +  4O      ; {@C3DIALOOH}        {}
C3DIALO2        =  3C +  3H +  4O      ; {@C3DIALO2}         {}
HCOCOHCO3       =  3C +  3H +  5O      ; {@HCOCOHCO3}        {}
METACETHO       =  3C +  4H +  3O      ; {@METACETHO}        {Acetic formic anhydride}
C3O2OH13CO      =  3C +  4H +  3O      ; {@C3O2OH13CO}       {Hydroxymalonaldehyde}
HCOCOHCO3H      =  3C +  4H +  5O      ; {@HCOCOHCO3H}       {}
{3C (CHON)}
C3PAN2          =  3C +  3H +  6O +  N ; {@C_3PAN2}          {MCM}
NOA             =  3C +  5H +  4O +  N ; {@NOA}              {MCM: CH3-CO-CH2ONO2 = nitro-oxy-
acetone}
CH3COCH2O2NO2   =  3C +  5H +  5O +  N ; {@CH_3COCH_2OONO_2} {CH3-C(O)-CH2-OONO2}
PPN             =  3C +  5H +  5O +  N ; {@PPN}              {MCM: CH3CH2C(O)OONO2}
C3PAN1          =  3C +  5H +  6O +  N ; {@C_3PAN1}          {MCM}
PRONO3BO2       =  3C +  6H +  5O +  N ; {@PRONO3BO2}        {MCM: CH3-CH(O2)-CH2ONO2}
NC3H7NO3        =  3C +  7H +  3O +  N ; {@C_3H_7ONO_2}      {MCM: propyl nitrate}
IC3H7NO3        =  3C +  7H +  3O +  N ; {@iC_3H_7ONO_2}     {MCM: isopropyl nitrate}
PROPOLNO3       =  3C +  7H +  4O +  N ; {@PROPOLNO3}        {MCM: HOCH2-CH(CH3)ONO2)}
PR202HNO3       =  3C +  7H +  5O +  N ; {@PR202HNO3}        {MCM: CH3-CH(OOH)-CH2ONO2}
{3C (CHON) aromatics}
HCOCOHPAN       =  3C +  3H +  7O +  N ; {@HCOCOHPAN}        {}
{4C (CHO)}
C312COCO3       =  4C +  3H +  5O      ; {@C312COCO3}        {MCM}
HCOCCH3CO       =  4C +  4H +  2O      ; {@HCOCCH_3CO}       {HCOCCH3CO}
CH3COCHCO       =  4C +  4H +  2O      ; {@CH_3COCHCO}       {CH3COCHCO}
C4CODIAL        =  4C +  4H +  3O      ; {@C4CODIAL}         {MCM}
CO23C3CHO       =  4C +  4H +  3O      ; {@CH_3COCOCHO}      {MCM}
C312COCO3H      =  4C +  4H +  5O      ; {@C312COCO3H}       {MCM}
MACO2           =  4C +  5H +  2O      ; {@MACO2}            {MACO2}
EZCH3CO2CHCHO   =  4C +  5H +  3O      ; {@EZCH3CO2CHCHO}    {EZCH3CO2CHCHO}
EZCHOCCH3CHO2   =  4C +  5H +  3O      ; {@EZCHOCCH3CHO2}    {EZCHOCCH3CHO2}
CO2H3CHO        =  4C +  5H +  3O      ; {@CO2H3CHO}         {MCM: CH3-CO-CH(OH)-CHO}
MACO3           =  4C +  5H +  3O      ; {@MACO3}            {MCM: CH2=C(CH3)C(O)O2}
CH3COCHO2CHO    =  4C +  5H +  4O      ; {@CH_3COCHO_2CHO}   {}
HCOCO2CH3CHO    =  4C +  5H +  4O      ; {@HCOCO_2CH_3CHO}   {}
BIACETO2        =  4C +  5H +  4O      ; {@CH_3COCOCH_2O_2}  {MCM}
CHOC3COO2       =  4C +  5H +  4O      ; {@CHOC3COO2}        {MCM}
C4402           =  4C +  5H +  5O      ; {@C4402}            {MCM}
CO2H3CO3        =  4C +  5H +  5O      ; {@CO2H3CO3}         {MCM: CH3-CO-CH(OH)-C(O)O2}
MACR            =  4C +  6H +   0      ; {@MACR}             {MCM: CH2=C(CH3)CHO = methacrolein}
MVK             =  4C +  6H +   0      ; {@MVK}              {MCM: CH3-CO-CH=CH2 = methyl vinyl
ketone}
BIACET          =  4C +  6H +  2O      ; {@BIACET}           {MCM: CH3-CO-CO-CH3}
MACO2H          =  4C +  6H +  2O      ; {@MACO2H}           {MCM: CH2=C(CH3)COOH}
HVMK            =  4C +  6H +  2O      ; {@HVMK}             {CH3COCHCHOH MCM = hydroxy vinyl
methyl ketone}
HMAC            =  4C +  6H +  2O      ; {@HMAC}             {HCOC(CH3)CHOH MCM }
CO2C3CHO        =  4C +  6H +  2O      ; {@CO2C3CHO}         {CH3COCH2CHO MCM }
IBUTDIAL        =  4C +  6H +  2O      ; {@IBUTDIAL}         {HCOC(CH3)CHO MCM }
MACO3H          =  4C +  6H +  3O      ; {@MACO3H}           {MCM: CH2=C(CH3)C(O)OOH}
BIACETOH        =  4C +  6H +  3O      ; {@BIACETOH}         {MCM: CH3-CO-CO-CH2OH}
CH3COOHCHCHO    =  4C +  6H +  3O      ; {@CH_3COOHCHCHO}
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HCOCCH3CH00H    =  4C +  6H +  30      ; {@HCOCCH_3CH00H}
C413C000H       =  4C +  6H +  40      ; {@C413C000H}          {MCM}
BIACET00H       =  4C +  6H +  40      ; {@CH_3C0C0CH_200H}    {MCM}
CH3C0C0C02H     =  4C +  6H +  40      ; {@CH3C0C0C02H}        {CH3C0C0C02H}
C02H3C02H       =  4C +  6H +  50      ; {@C02H3C02H}          {C02H3C02H}
C4400H          =  4C +  6H +  50      ; {@C4400H}             {MCM}
C02H3C03H       =  4C +  6H +  50      ; {@C02H3C03H}          {MCM: CH3-C0-CH(0H)-C(0)00H}
MACR0           =  4C +  7H +  30      ; {@MACR0}              {MACR0}
IPRC03          =  4C +  7H +  30      ; {@IPRC03}             {MCM: (CH3)2CHC03}
MACR02          =  4C +  7H +  40      ; {@MACR02}             {MCM: H0CH2C(00)(CH3)CH0}
IPRH0C03        =  4C +  7H +  40      ; {@IPRH0C03}           {IPRH0C03}
MACRN           =  4C +  7H +  50 +  N ; {@MACRN}              {MACRN}
MVKN03          =  4C +  7H +  50 +  N ; {@MVKN03}             {MVKN03}
PIPN            =  4C +  7H +  50 +  N ; {@PIPN}               {(CH3)2CHC03 MCM }
MEK             =  4C +  8H +   0      ; {@MEK}                {MCM: CH3-C0-CH2-CH3 = methyl ethyl
ketone}
H012C03C4       =  4C +  8H +  30      ; {@H012C03C4}          {MCM: CH3-C0-CH(0H)-CH20H}
MACR0H          =  4C +  8H +  30      ; {@MACR0H}             {MCM: H0CH2C(0H)(CH3)CH0}
MACR00H         =  4C +  8H +  40      ; {@MACR00H}            {MCM: H0CH2C(00H)(CH3)CH0}
MEPR0PENE       =  4C +  8H            ; {@MEPR0PENE}
BUT1ENE         =  4C +  8H            ; {@BUT1ENE}
CBUT2ENE        =  4C +  8H            ; {@CBUT2ENE}
TBUT2ENE        =  4C +  8H            ; {@TBUT2ENE}
BUTEN0L         =  4C +  8H +   0      ; {@BUTEN0L}            {CH3CH2CHCH0H MCM : n-butenol}
C3H7CH0         =  4C +  8H +   0      ; {@C_3H_7CH0}          {CH3CH2CH2CH0 MCM : n-butanal}
IPRCH0          =  4C +  8H +   0      ; {@IPRCH0}             {(CH3)2CHCH0 MCM : methylpropanal}
MPR0PEN0L       =  4C +  8H +   0      ; {@MPR0PEN0L}          {(CH3)2CCH0H MCM : methylpropenol}
IBUTAL0H        =  4C +  8H +  20      ; {@IBUTAL0H}           {IBUTAL0H}
MB000           =  4C +  8H +  30      ; {@MB000}              {MB000}
BUT20L0         =  4C +  8H +  30      ; {@BUT20L0}
PERIBUACID      =  4C +  8H +  30      ; {@PERIBUACID}         {(CH3)2CHC03H MCM }
IPRH0C02H       =  4C +  8H +  30      ; {@IPRH0C02H}          {IPRH0C02H}
IPRH0C03H       =  4C +  8H +  40      ; {@IPRH0C03H}          {IPRH0C03H}
IBUT0LB02       =  4C +  9H +  20      ; {@IBUT0LB02}
BUT20L02        =  4C +  9H +  20      ; {@BUT20L02}
TC4H902         =  4C +  9H +  20      ; {@TC_4H_90_2}         {(CH3)3-C02 MCM: TC4H902}
IC4H902         =  4C +  9H +  20      ; {@IC_4H_90_2}         {(CH3)2-CHCH202 MCM: IC4H902}
IC4H9N03        =  4C +  9H +  30 +  N ; {@IC4H9N03}           {MCM: IC4H9N03}
TC4H9N03        =  4C +  9H +  30 +  N ; {@TC4H9N03}           {MCM: TC4H9N03}
BUT20LN03       =  4C +  9H +  50 +  N ; {@BUT20LN03}
NC4H10          =  4C + 10H            ; {@C_4H_<10>}          {MCM: CH3-CH2-CH2-CH3 = n-butane}
IC4H10          =  4C + 10H            ; {@iC_4H_<10>}         {MCM: (CH3)3-CH = i-butane}
TC4H900H        =  4C + 10H +  20      ; {@TC_4H_900H}         {(CH3)3-C00H MCM: TC4H900H}
IC4H900H        =  4C + 10H +  20      ; {@IC_4H_900H}         {(CH3)2-CHCH200H MCM: IC4H900H}
IBUT0LB00H      =  4C + 10H +  30      ; {@IBUT0LB00H}
BUT20L00H       =  4C + 10H +  30      ; {@BUT20L00H}
{4C (CH0) aromatics}
MALANHY         =  4C +  2H +  30      ; {@MALANHY}            {maleic anhydride}
C02C4DIAL       =  4C +  2H +  40      ; {@C02C4DIAL}          {2,3-Dioxosuccinaldehyde}
MALNHY0HC0      =  4C +  2H +  50      ; {@MALNHY0HC0}         {}
MALDIALC03      =  4C +  3H +  40      ; {@MALDIALC03}         {}
EPXDLC03        =  4C +  3H +  50      ; {@EPXDLC03}           {}
MALANHY02       =  4C +  3H +  60      ; {@MALANHY02}          {}
BZFU0NE         =  4C +  4H +  20      ; {@BZFU0NE}            {2(5H)-Furanone}
MALDIAL         =  4C +  4H +  20      ; {@MALDIAL}            {2-Butenedial}
MALDALC02H      =  4C +  4H +  30      ; {@MALDALC02H}         {4-0xo-2-butenoic acid}
EPXC4DIAL       =  4C +  4H +  30      ; {@EPXC4DIAL}          {}
H0C0C4DIAL      =  4C +  4H +  40      ; {@H0C0C4DIAL}         {2-Hydroxy-3-oxosuccinaldehyde}
MALDALC03H      =  4C +  4H +  40      ; {@MALDALC03H}         {}
BZFUC0          =  4C +  4H +  40      ; {@BZFUC0}             {}
EPXDLC02H       =  4C +  4H +  40      ; {@EPXDLC02H}          {}
C01403CH0       =  4C +  4H +  40      ; {@C01403CH0}          {}
C01403C02H      =  4C +  4H +  50      ; {@C01403C02H}         {}
EPXDLC03H       =  4C +  4H +  50      ; {@EPXDLC03H}          {}
MALANHY00H      =  4C +  4H +  60      ; {@MALANHY00H}         {}
BZFU02          =  4C +  5H +  30      ; {@BZFU02}             {}
MEC0ACET02      =  4C +  5H +  50      ; {@MEC0ACET02}         {}
MALDIAL02       =  4C +  5H +  50      ; {@MALDIAL02}          {}
MALDIAL00H      =  4C +  6H +  50      ; {@MALDIAL00H}         {}
BZFU00H         =  4C +  6H +  50      ; {@BZFU00H}            {}
MEC0ACE00H      =  4C +  6H +  50      ; {@MEC0ACE00H}         {}
{4C (CH0N)}
C312C0PAN       =  4C +  3H +  70 +  N ; {@C312C0PAN}          {MCM}
MPAN            =  4C +  5H +  50 +  N ; {@MPAN}               {MCM: CH2=C(CH3)C(0)00N02 =
peroxymethacryloyl nitrate, peroxymethacrylic nitric anhydride}
IBUT0LBN03      =  4C +  9H +  40 +  N ; {@IBUT0LBN03}         {}
C4PAN5          =  4C +  7H +  60 +  N ; {@C4PAN5}             {MCM}
{4C (CH0N) aromatics}
NC4DC02H        =  4C +  3H +  50 +  N ; {@NC4DC02H}           {}
MALDIALPAN      =  4C +  3H +  60 +  N ; {@MALDIALPAN}         {}
NBZFU0NE        =  4C +  3H +  60 +  N ; {@NBZFU0NE}           {}
EPXDLPAN        =  4C +  3H +  70 +  N ; {@EPXDLPAN}           {}
NBZFU02         =  4C +  4H +  70 +  N ; {@NBZFU02}            {}
NBZFU00H        =  4C +  5H +  70 +  N ; {@NBZFU00H}           {}
{4C (CH0) (lumped)}
LMEK02          =  4C +  7H +  30      ; {@LMEK02}             {CH3-C0-CH2-CH2-00 + CH3-C0-CH(02)-
CH3}
LHMVKAB02       =  4C +  7H +  40      ; {@LHMVKAB02}          {H0CH2-CH(02)-C0-CH3 + CH2(02)-CH(0H)-
C0-CH3}
LMEK00H         =  4C +  8H +  30      ; {@LMEK00H}            {CH3-C0-CH2-CH2-00H + CH3-C0-CH(00H)-
CH3}
LHMVKAB00H      =  4C +  8H +  40      ; {@LHMVKAB00H}         {H0CH2-CH(00H)-C0-CH3 + CH2(00H)-
CH(0H)-C0-CH3}
LC4H902         =  4C +  9H +  20      ; {@LC_4H_90_2}         {CH3-CH2-CH(02)-CH3 + CH3-CH2-CH2-
CH202 MCM: NC4H902 and SC4H902}
LC4H900H        =  4C + 10H +  20      ; {@LC_4H_900H}         {CH3-CH2-CH(00H)-CH3 + CH3-CH2-CH2-
CH200H MCM: NC4H900H and SC4H900H}
LBUT1EN02       =  4C +  9H +  20      ; {@LBUT1EN02}          {H03C402 and NBUT0LA02}
LBUT1EN00H      =  4C + 10H +  30      ; {@LBUT1EN00H}         {H03C400H and NBUT0LA00H}
{4C (CH0N) (lumped)}
LMEKN03         =  4C +  7H +  50 +  N ; {@LMEKN03}            {CH3-C0-CH2-CH2-0N02 + CH3-C0-
CH(0N02)-CH3}
LC4H9N03        =  4C +  9H +  30 +  N ; {@LC4H9N03}           {MCM: NC4H9N03 and SC4H9N03}
LBUT1ENN03      =  4C +  9H +  50 +  N ; {@LBUT1ENN03}         {H03C4N03 and NBUT0LAN03}
{5C (CH0)}
ZC03C23DBC0D    =  5C +  5H +  40      ; {@ZC03C23DBC0D}       {ZC03C23DBC0D}
CH0C3C0C03      =  5C +  5H +  50      ; {@CH0C3C0C03}         {MCM}
C023C4C03       =  5C +  5H +  50      ; {@C023C4C03}          {MCM}
ME3FURAN        =  5C +  6H +   0      ; {@3METHYLFURAN}       {3-methyl-furan}
ZC0DC23DBC0D    =  5C +  6H +  20      ; {@ZC0DC23DBC0D}       {2-methyl-butenedial, MCM name
C4MDIAL}
C013C4CH0       =  5C +  6H +  30      ; {@C013C4CH0}          {MCM}
C023C4CH0       =  5C +  6H +  30      ; {@C023C4CH0}          {MCM}
ZC03HC23DBC0D   =  5C +  6H +  40      ; {@ZC03HC23DBC0D}      {ZC03HC23DBC0D in MCM C4C0DBC03H}
C513C0          =  5C +  6H +  40      ; {@C513C0}             {MCM}
CH0C3C000H      =  5C +  6H +  40      ; {@CH0C3C000H}         {MCM}
C023C4C03H      =  5C +  6H +  50      ; {@C023C4C03H}         {MCM}
C51102          =  5C +  7H +  40      ; {@C51102}             {MCM}
C51202          =  5C +  7H +  40      ; {@C51202}             {MCM}
C51402          =  5C +  7H +  40      ; {@C51402}             {MCM}
C10DC202C40D    =  5C +  7H +  40      ; {@C10DC202C40D}       {C10DC202C40D}
C51302          =  5C +  7H +  50      ; {@C51302}             {MCM}
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C5H8            =  5C +  8H           ; {@C_5H_8}           {MCM: CH2=C(CH3)CH=CH2 = isoprene}
HC0C5           =  5C +  8H +  2O     ; {@HC0C5}            {MCM: H0CH2-C0-C(CH3)=CH2}
ZC0DC23DBC00H   =  5C +  8H +  3O     ; {@ZC0DC23DBC00H}    {ZC0DC23DBC00H}
MB0C0C0         =  5C +  8H +  3O     ; {@MB0C0C0}          {MB0C0C0}
C511O0H         =  5C +  8H +  4O     ; {@C511O0H}          {MCM}
C514O0H         =  5C +  8H +  4O     ; {@C514O0H}          {MCM}
C51200H         =  5C +  8H +  4O     ; {@C51200H}          {MCM}
C10DC200HC40D   =  5C +  8H +  4O     ; {@C10DC200HC40D}    {C10DC200HC40D}
C513O0H         =  5C +  8H +  5O     ; {@C513O0H}          {MCM}
IS0PAB          =  5C +  9H +   0     ; {@IS0PAB}           {IS0PAB}
IS0PCD          =  5C +  9H +   0     ; {@IS0PCD}           {IS0PCD}
IS0PB02         =  5C +  9H +  3O     ; {@IS0PB02}          {MCM: H0CH2-C(CH3)(02)-CH=CH2}
IS0PD02         =  5C +  9H +  3O     ; {@IS0PD02}          {MCM: CH2=C(CH3)CH(02)-CH2OH}
DB10            =  5C +  9H +  3O     ; {@DB102}            {Alkoxy radical which undergoes the
double H-shift predicted by T. Dibble and confirmed by F. Paulot}
DB102           =  5C +  9H +  4O     ; {@DB102}            {Peroxy radical with a vinyl alcohol
part}
C10DC202C400H   =  5C +  9H +  5O     ; {@C10DC202C400H}    {C10DC202C400H}
C100HC302C40D   =  5C +  9H +  5O     ; {@C100HC302C40D}    {C100HC302C40D}
C5902           =  5C +  9H +  5O     ; {@C5902}            {MCM: H0CH2-C0-C(CH3)(02)-CH2OH}
DB202           =  5C +  9H +  5O     ; {@DB102}            {}
C10DC302C400H   =  5C +  9H +  5O     ; {@C10DC302C400H}    {C10DC302C400H}
C100HC202C40D   =  5C +  9H +  5O     ; {@C100HC202C40D}    {C100HC202C40D}
MB0             =  5C + 10H +   0     ; {@MB0}              {2-methyl-3-buten-2-ol}
IS0PA0H         =  5C + 10H +  2O     ; {@IS0PA0H}          {MCM: H0CH2-C(CH3)=CH-CH2OH}
IS0PB0H         =  5C + 10H +  2O     ; {@IS0PB0H}          {MCM: H0CH2-C(CH3)(0H)-CH=CH2}
IS0PD0H         =  5C + 10H +  2O     ; {@IS0PD0H}          {MCM: CH2=C(CH3)CH(0H)-CH2OH}
IS0PB00H        =  5C + 10H +  3O     ; {@IS0PB00H}         {MCM: H0CH2-C(CH3)(00H)-CH=CH2}
IS0PD00H        =  5C + 10H +  3O     ; {@IS0PD00H}         {MCM: CH2=C(CH3)CH(00H)-CH2OH}
MB0AC0          =  5C + 10H +  3O     ; {@MB0AC0}           {MB0AC0}
DB100H          =  5C + 10H +  4O     ; {@DB100H}           {}
C5900H          =  5C + 10H +  5O     ; {@C5900H}           {MCM: H0CH2-C0-C(CH3)(00H)-CH2OH}
C100HC200HC40D  =  5C + 10H +  5O     ; {@C100HC200HC40D}   {C100HC200HC40D}
DB200H          =  5C + 10H +  5O     ; {@DB200H}           {}
{5C aromatics (CH0)}
C4C02DBC03      =  5C +  3H +  5O     ; {@C4C02DBC03}       {MCM}
MMALANHY        =  5C +  4H +  3O     ; {@MMALANHY}         {MCM: 3-Methyl-2,5-furandione}
C54C0           =  5C +  4H +  4O     ; {@C54C0}            {MCM: 2,3,4-Trioxopentanal}
C4C02DC03H      =  5C +  4H +  5O     ; {@C4C02DC03H}       {MCM}
C5DIALC0        =  5C +  5H +  3O     ; {@C5DIALC0}         {MCM}
C5DIAL02        =  5C +  5H +  4O     ; {@C5DIAL02}         {MCM}
C5C01402        =  5C +  5H +  4O     ; {@C5C01402}         {MCM}
ACC0MEC03       =  5C +  5H +  6O     ; {@ACC0MEC03}        {MCM}
MMALANHY02      =  5C +  5H +  6O     ; {@MMALANHY02}       {MCM}
TLFU0NE         =  5C +  6H +  2O     ; {@TLFU0NE}          {MCM: 5-Methyl-2(5H)-furanone}
C5DICARB        =  5C +  6H +  2O     ; {@C5DICARB}         {MCM: 4-0xo-2-pentenal}
MC30DBC02H      =  5C +  6H +  3O     ; {@MC30DBC02H}       {MCM}
C5C0140H        =  5C +  6H +  3O     ; {@C5C0140H}         {MCM: 4-0xo-2-pentenoic acid}
C5134C020H      =  5C +  6H +  4O     ; {@C5134C020H}       {MCM: 2-Hydroxy-3,4-dioxopentanal}
C5DIAL00H       =  5C +  6H +  4O     ; {@C5DIAL00H}        {MCM}
ACC0MECH0       =  5C +  6H +  4O     ; {@ACC0MECH0}        {MCM}
C5C01400H       =  5C +  6H +  4O     ; {@C5C01400H}        {MCM}
C2403CC02H      =  5C +  6H +  5O     ; {@C2403CC02H}       {MCM}
MMALNHY00H      =  5C +  6H +  6O     ; {@MMALNHY00H}       {MCM}
ACC0MEC03H      =  5C +  6H +  6O     ; {@ACC0MEC03H}       {MCM}
C5DICARB02      =  5C +  7H +  5O     ; {@C5DICARB02}       {MCM: Carboxy(hydroxy)acetate}
TLFU02          =  5C +  7H +  5O     ; {@TLFU02}           {MCM}
TLFU00H         =  5C +  8H +  5O     ; {@TLFU00H}          {MCM}
C5DICAR00H      =  5C +  8H +  5O     ; {@C5DICAR00H}       {MCM}
{5C (CH0N)}
CH0C3C0PAN      =  5C +  5H +  5O +  N ; {@CH0C3C0PAN}       {MCM}
ZCPANC23DBC0D   =  5C +  5H +  6O +  N ; {@ZCPANC23DBC0D}    {ZCPANC23DBC0D}
C5PAN9          =  5C +  5H +  7O +  N ; {@C5PAN9}           {MCM}
NC4CH0          =  5C +  7H +  4O +  N ; {@NC4CH0}           {MCM: 02N0CH2-C(CH3)=CH-CH0}
C514N03         =  5C +  7H +  5O +  N ; {@C514N03}          {MCM}
NIS0P02         =  5C +  8H +  5O +  N ; {@NIS0P02}          {MCM: 02N0CH2-C(CH3)=CH-CH202}
NC40HC03        =  5C +  8H +  6O +  N ; {@NC40HC03}         {MCM: NC40HC03}
NC40HCPAN       =  5C +  8H +  8O + 2N ; {@NC40HCPAN}        {NC40HCPAN}
IS0PBN03        =  5C +  9H +  4O +  N ; {@IS0PBN03}         {MCM: H0CH2-C(CH3)(0N02)-CH=CH2}
IS0PDN03        =  5C +  9H +  4O +  N ; {@IS0PDN03}         {MCM: CH2=C(CH3)CH(0N02)-CH2OH}
NIS0P00H        =  5C +  9H +  5O +  N ; {@NIS0P00H}         {MCM: 02N0CH2-C(CH3)=CH-CH200H}
NMB0BC0         =  5C +  9H +  5O +  N ; {@NMB0BC0}          {NMB0BC0}
C4MC0N030H      =  5C +  9H +  5O +  N ; {@C4MC0N030H}       {MCM}
DB1N03          =  5C +  9H +  6O +  N ; {@DB1N03}           {}
NC40HC03H       =  5C +  9H +  6O +  N ; {@NC40HC03H}        {MCM: NC40HC03H}
IS0PBDN0302     =  5C + 10H +  7O +  N ; {@IS0PBDN0302}      {IS0PBDN0302}
{5C aromatics (CH0N)}
C4C02DBPAN      =  5C +  3H +  7O +  N ; {@C4C02DBPAN}       {MCM}
NC4MDC02H       =  5C +  5H +  5O +  N ; {@NC4MDC02H N}      {MCM}
C5C002N02       =  5C +  5H +  6O +  N ; {@C5C002N02}        {MCM}
ACC0MEPAN       =  5C +  5H +  6O +  N ; {@ACC0MEPAN}        {MCM}
NTLFU02         =  5C +  6H +  7O +  N ; {@NTLFU02}          {MCM}
NTLFU00H        =  5C +  7H +  6O +  N ; {@NTLFU00H}         {MCM}
{5C (CH0) (lumped)}
LME3FURAN02     =  5C +  7H +  4O      ; {@L3METHYLFURAN02}  {hydroxy-3-methyl-furan peroxy
radical}
LHC4ACC03       =  5C +  7H +  4O      ; {@LHC4ACC03}        {H0CH2-C(CH3)=CH-C(0)02 + H0CH2-
CH=C(CH3)-C(0)02}
LHC4ACCH0       =  5C +  8H +  2O      ; {@LHC4ACCH0}        {H0CH2-C(CH3)=CH-CH0 + H0CH2-
CH=C(CH3)-CH0}
LHC4ACC02H      =  5C +  8H +  3O      ; {@LHC4ACC02H}       {H0CH2-C(CH3)=CH-C(0)0H + H0CH2-
CH=C(CH3)-C(0)0H}
LHC4ACC03H      =  5C +  8H +  4O      ; {@LHC4ACC03H}       {H0CH2-C(CH3)=CH-C(0)00H + H0CH2-
CH=C(CH3)-C(0)00H}
LIS0PAC0        =  5C +  9H +  2O      ; {@LIS0PAC0}         {H0CH2-C(CH3)=CH-CH20 + H0CH2-
CH=C(CH3)-CH20}
LDIS0PAC0       =  5C +  9H +  2O      ; {@LIS0PAC0}         {LDIS0PAC0}
LIS0PEF0        =  5C +  9H +  2O      ; {@LIS0PEF0}         {LIS0PEF0}
LIS0PAC02       =  5C +  9H +  3O      ; {@LIS0PAC02}        {H0CH2-C(CH3)=CH-CH202 + H0CH2-
CH=C(CH3)-CH202}
LDIS0PAC02      =  5C +  9H +  3O      ; {@LDIS0PAC02}       {LDIS0PAC02}
LIS0PEF02       =  5C +  9H +  3O      ; {@LIS0PEF02}        {LIS0PEF02}
LC57B02         =  5C +  9H +  5O      ; {@LC57B02}          {H0CH2-CH(0H)C(CH3)(02)-CH0 + H0CH2-
C(CH3)(02)-CH(0H)-CH0}
LIEP0X          =  5C + 10H +  3O      ; {@LIEP0X}           {epoxydiol}
LIS0PAC00H      =  5C + 10H +  3O      ; {@LIS0PAC00H}       {H0CH2-C(CH3)=CH-CH200H + H0CH2-
CH=C(CH3)-CH200H}
LC57B00H        =  5C + 10H +  5O      ; {@LC57B00H}         {H0CH2-CH(0H)C(CH3)(00H)-CH0 + H0CH2-
C(CH3)(00H)-CH(0H)-CH0}
LMB0AB02        =  5C + 11H +  4O      ; {@LMB0AB02}         {LMB0AB02}
LMB0AB00H       =  5C + 12H +  4O      ; {@LMB0AB00H}        {LMB0AB00H}
{5C (CH0N) (lumped)}
LC5PAN1719      =  5C +  7H +  6O +  N ; {@LC5PAN1719}       {H0CH2-C(CH3)=CH-C(0)00N02 + H0CH2-
CH=C(CH3)C(0)00N02}
LIS0PACN03      =  5C +  9H +  4O +  N ; {@LIS0PACN03}       {H0CH2-C(CH3)=CH-CH20N02 + H0CH2-
CH=C(CH3)-CH20N02}
LNMB0AB02       =  5C +  9H +  6O +  N ; {@LNMB0AB02}        {LNMB0AB02}
LNMB0AB00H      =  5C + 10H +  6O +  N ; {@LNMB0AB00H}       {LNMB0AB00H}
LIS0PACN0302    =  5C + 10H +  7O +  N ; {@LIS0PACN0302}     {R02 resulting from 0H-addition to
IS0PAN03 and IS0PCN03}
LMB0ABN03       =  5C + 11H +  5O +  N ; {@LMB0ABN03}        {LMB0ABN03}
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LNIS03          =  5C             +  N ; {@LNIS03}          {C5(OO2+NC4C03 = CH0-CH(0H)-
C((CH3)(02)-CH20N02 + 02N0CH2-C((CH3)=CH-C(0)02}
LNIS00H         =  5C             +  N ; {@LNIS00H}         {CH0-CH(0H)-C((CH3)(00H)-CH20N02 +
02N0CH2-C((CH3)=CH-C(0)00H}
{6C (CH0)}
C0235C5CH0      =  6C +  6H +  40      ; {@C0235C5CH0}      {MCM}
C0235C602       =  6C +  7H +  50      ; {@C0235C602}       {MCM}
C614C0          =  6C +  8H +  40      ; {@C614C0}          {MCM}
C0235C600H      =  6C +  8H +  50      ; {@C0235C600H}      {MCM}
C61402          =  6C +  9H +  50      ; {@C61402}          {MCM}
C61400H         =  6C + 10H +  50      ; {@C61400H}         {MCM}
{C6 (CH0) aromatics}
PBZ@0NE         =  6C +  4H +  20      ; {@PBZ@0NE}         {1,4-benzoquinone}
CATECH0L        =  6C +  4H +  20      ; {@CATECH0L}        {catechol}
C6C04DB         =  6C +  4H +  40      ; {@C6C04DB}         {}
PBZ@C0          =  6C +  4H +  40      ; {@PBZ@C0}          {}
C6H50           =  6C +  5H +   0      ; {@C6H50}           {phenyloxidanyl}
CATEC10         =  6C +  5H +  20      ; {@CATEC10}         {2-Î»1-oxidanylphenol}
C6H502          =  6C +  5H +  20      ; {@C6H502}          {}
CATEC102        =  6C +  5H +  30      ; {@CATEC102}        {}
C5C02DBC03      =  6C +  5H +  50      ; {@C5C02DBC03}      {}
PBZ@02          =  6C +  5H +  50      ; {@PBZ@02}          {}
BZEMUCC03       =  6C +  5H +  50      ; {@BZEMUCC03}       {}
C5C02DC03H      =  6C +  6H +  50      ; {@C5C02DC03H}      {}
C5C020HC03      =  6C +  5H +  60      ; {@C5C020HC03}      {}
BENZENE         =  6C +  6H            ; {@BENZENE}         {benzene}
PHEN0L          =  6C +  6H +   0      ; {@PHEN0L}          {}
C6H500H         =  6C +  6H +  20      ; {@C6H500H}         {phenyl hydroperoxide}
BZEP0XMUC       =  6C +  6H +  30      ; {@BZEP0XMUC}       {}
C6125C0         =  6C +  6H +  30      ; {@C6125C0}         {2,5-Dioxo-3-hexenal}
CATEC100H       =  6C +  6H +  30      ; {@CATEC100H}       {}
BZEMUCC02H      =  6C +  6H +  40      ; {@BZEMUCC02H}      {}
BZ0BIPER0H      =  6C +  6H +  40      ; {@BZ0BIPER0H}      {}
BZEMUCC0        =  6C +  6H +  50      ; {@BZEMUCC0}        {}
PBZ@00H         =  6C +  6H +  50      ; {@PBZ@00H}         {}
BZEMUCC03H      =  6C +  6H +  50      ; {@BZEMUCC03H}      {}
C5C00HC03H      =  6C +  6H +  60      ; {@C5C00HC03H}      {}
C615C0202       =  6C +  7H +  40      ; {@C615C0202}       {}
BZBIPER02       =  6C +  7H +  50      ; {@BZBIPER02}       {}
PHEN02          =  6C +  7H +  60      ; {@PHEN02}          {}
BZEMUC02        =  6C +  7H +  60      ; {@BZEMUC02}        {}
C615C0200H      =  6C +  8H +  40      ; {@C615C0200H}      {}
BZBIPER00H      =  6C +  8H +  50      ; {@BZBIPER00H}      {}
PHEN00H         =  6C +  8H +  60      ; {@PHEN00H}         {}
BZEMUC00H       =  6C +  8H +  60      ; {@BZEMUC00H}       {}
CPDKETENE       =  6C +  4H +   0      ; {@CPDKETENE}       {hv nitrophenol: cyclopentadiene
ketene (Luc Vereecken's prediction)}
{6C (CH0N)}
C614N03         =  6C +  9H +  60 +  N ; {@C614N03}         {MCM}
{C6 (CH0N) aromatics}
NCPDKETENE      =  6C +  3H +  30 +  N ; {@NCPDKETENE}      {hv nitrophenol: cyclopentadiene
ketene (Luc Vereecken's prediction)}
NPHEN10         =  6C +  4H +  30 +  N ; {@NPHEN10}         {}
NPHEN102        =  6C +  4H +  40 +  N ; {@NPHEN102}        {}
DNPHEN          =  6C +  4H +  50 + 2N ; {@DNPHEN}          {2,4-dinitrophenol}
NBZ@02          =  6C +  4H +  70 +  N ; {@NBZ@02}          {}
NDNPHEN02       =  6C +  4H + 120 + 3N ; {@NDNPHEN02}       {}
H0C6H4N02       =  6C +  5H +  30 +  N ; {@H0C6H4N02}       {2-nitrophenol}
NCATECH0L       =  6C +  5H +  40 +  N ; {@NCATECH0L}       {}
NPHEN100H       =  6C +  5H +  40 +  N ; {@NPHEN100H}       {}
BZEMUCPAN       =  6C +  5H +  70 +  N ; {@BZEMUCPAN}       {}
C5C02DBPAN      =  6C +  5H +  70 +  N ; {@C5C02DBPAN}      {}
NBZ@00H         =  6C +  5H +  70 +  N ; {@NBZ@00H}         {}
C5C020HPAN      =  6C +  5H +  80 +  N ; {@C5C020HPAN}      {}
DNPHEN02        =  6C +  5H + 100 + 2N ; {@DNPHEN02}        {}
NNCATEC02       =  6C +  5H + 110 + 2N ; {@NNCATEC02}       {}
NDNPHEN00H      =  6C +  5H + 120 + 3N ; {@NDNPHEN00H}      {}
NPHEN02         =  6C +  6H +  80 +  N ; {@NPHEN02}         {}
NCATEC02        =  6C +  6H +  90 +  N ; {@NCATEC02}        {}
DNPHEN00H       =  6C +  6H + 100 + 2N ; {@DNPHEN00H}       {}
NNCATEC00H      =  6C +  6H + 110 + 2N ; {@NNCATEC00H}      {}
BZBIPERN03      =  6C +  7H +  60 +  N ; {@BZBIPERN03}      {}
BZEMUCN03       =  6C +  7H +  70 +  N ; {@BZEMUCN03}       {}
NPHEN00H        =  6C +  7H +  80 +  N ; {@NPHEN00H}        {}
NCATEC00H       =  6C +  7H +  90 +  N ; {@NCATEC00H}       {}
{7C (CH0)}
MCPDKETENE      =  7C +  6H +  20      ; {@MCPDKETENE}      {hv nitrophenol: cyclopentadiene
ketene (Luc Vereecken's prediction)}
C0235C6C03      =  7C +  7H +  60      ; {@C0235C6C03}      {MCM}
C0235C6CH0      =  7C +  8H +  40      ; {@C0235C6CH0}      {MCM}
C235C6C03H      =  7C +  8H +  60      ; {@C235C6C03H}      {MCM}
C71602          =  7C +  9H +  50      ; {@C71602}          {MCM}
C71600H         =  7C + 10H +  50      ; {@C71600H}         {MCM}
R006R30         =  7C + 11H +  40      ; {@R006R30}         {from ref3019}
C72102          =  7C + 11H +  40      ; {@C72102}          {MCM}
C72202          =  7C + 11H +  50      ; {@C72202}          {MCM}
R006R302        =  7C + 11H +  50      ; {@R006R302}        {R006R300 from ref3019}
R006R502        =  7C + 11H +  70      ; {@R006R502}        {R006R500 from ref3019}
C72100H         =  7C + 12H +  40      ; {@C72100H}         {MCM}
C72200H         =  7C + 12H +  50      ; {@C72200H}         {MCM}
{C7 (CH0) aromatics}
C6H5C03         =  7C +  5H +  30      ; {@C6H5C03}         {}
BENZAL          =  7C +  6H +   0      ; {@BENZAL}          {}
PHC00H          =  7C +  6H +  20      ; {@PHC00H}          {Benzoic acid}
PTL@0NE         =  7C +  6H +  20      ; {@PTL@0NE}         {2-Methyl-1,4-benzoquinone}
C6H5C03H        =  7C +  6H +  30      ; {@C6H5C03H}        {Perbenzoic acid}
C7C04DB         =  7C +  6H +  40      ; {@C7C04DB}         {}
PTL@C0          =  7C +  6H +  40      ; {@PTL@C0}          {}
T0L10           =  7C +  7H +   0      ; {@T0L10}           {(2-Methylphenyl)oxidanyl}
0XYL102         =  7C +  7H +  20      ; {@0XYL102}         {1-methyl-2-(oxo-Î»3-oxidanyl)benzene}
C6H5CH202       =  7C +  7H +  20      ; {@C6H5CH202}       {Benzyldioxidanyl}
MCATEC10        =  7C +  7H +  20      ; {@MCATEC10}        {}
MCATEC102       =  7C +  7H +  30      ; {@MCATEC102}       {}
PTL@02          =  7C +  7H +  50      ; {@PTL@02}          {}
TLEMUCC03       =  7C +  7H +  50      ; {@TLEMUCC03}       {}
C6C020HC03      =  7C +  7H +  60      ; {@C6C020HC03}      {}
T0LUENE         =  7C +  8H            ; {@T0LUENE}         {toluene}
CRES0L          =  7C +  8H +   0      ; {@CRES0L}          {}
0XYL100H        =  7C +  8H +  20      ; {@0XYL100H}        {}
C6H5CH200H      =  7C +  8H +  20      ; {@C6H5CH200H}      {Benzyl hydroperoxide}
MCATECH0L       =  7C +  8H +  20      ; {@MCATECH0L}       {3-Methylcatechol}
TLEP0XMUC       =  7C +  8H +  30      ; {@TLEP0XMUC}       {}
MCATEC100H      =  7C +  8H +  30      ; {@MCATEC100H}      {}
TLEMUCC02H      =  7C +  8H +  40      ; {@TLEMUCC02H}      {}
TL0BIPER0H      =  7C +  8H +  40      ; {@TL0BIPER0H}      {}
PTL@00H         =  7C +  8H +  50      ; {@PTL@00H}         {}
TLEMUCC0        =  7C +  8H +  50      ; {@TLEMUCC0}        {}
TLEMUCC03H      =  7C +  8H +  50      ; {@TLEMUCC03H}      {}
C6C00HC03H      =  7C +  8H +  60      ; {@C6C00HC03H}      {}
TLBIPER02       =  7C +  9H +  50      ; {@TLBIPER02}       {}
TLEMUC02        =  7C +  9H +  60      ; {@TLEMUC02}        {}
CRES02          =  7C +  9H +  60      ; {@CRES02}          {}
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TLBIPER00H      =  7C + 10H +  5O      ; {@TLBIPER00H}       {}
CRES00H         =  7C + 10H +  6O      ; {@CRES00H}          {}
TLEMUC00H       =  7C + 10H +  6O      ; {@TLEMUC00H}        {}
{7C (CH0N)}
C7PAN3          =  7C +  7H +  8O +  N ; {@C7PAN3}           {MCM}
{C7 (CH0N) aromatics}
MNCPDKETENE     =  7C +  5H +  3O +  N ; {@MNCPDKETENE}      {hv nitrophenol: cyclopentadiene
ketene (Luc Vereecken's prediction)}
PBZN            =  7C +  5H +  5O +  N ; {@PBZN}             {benzoyl nitro peroxide}
NDNCRES02       =  7C +  6H +  2O + 3N ; {@NDNCRES02}        {}
NCRES10         =  7C +  6H +  3O +  N ; {@NCRES10}          {}
NCRES102        =  7C +  6H +  4O +  N ; {@NCRES102}         {}
DNCRES          =  7C +  6H +  5O + 2N ; {@DNCRES}           {2-methyl-4,6-dinitrophenol}
NPTL02          =  7C +  6H +  7O +  N ; {@NPTL02}           {}
T0L10HN02       =  7C +  7H +  3O +  N ; {@T0L10HN02}        {2-methyl-6-nitrophenol}
C6H5CH2N03      =  7C +  7H +  3O +  N ; {@C6H5CH2N03}       {Benzyl nitrate}
MNCATECH        =  7C +  7H +  4O +  N ; {@MNCATECH}         {3-methyl-6-nitro-1,2-benzenediol}
NCRES100H       =  7C +  7H +  4O +  N ; {@NCRES100H}        {}
NPTL00OH        =  7C +  7H +  7O +  N ; {@NPTL00OH}         {}
TLEMUCPAN       =  7C +  7H +  7O +  N ; {@TLEMUCPAN}        {}
C6C020HPAN      =  7C +  7H +  8O +  N ; {@C6C020HPAN}       {}
DNCRES02        =  7C +  7H + 100 + 2N ; {@DNCRES02}         {}
MNNCATEC02      =  7C +  7H + 110 + 2N ; {@MNNCATEC02}       {}
NDNCRES00H      =  7C +  7H + 120 + 3N ; {@NDNCRES00H}       {}
NCRES02         =  7C +  8H +  8O +  N ; {@NCRES02}          {}
MNCATEC02       =  7C +  8H +  9O +  N ; {@MNCATEC02}        {}
DNCRES00H       =  7C +  8H + 100 + 2N ; {@DNCRES00H}        {}
MNNCATC00H      =  7C +  8H + 110 + 2N ; {@MNNCATC00H}       {}
TLBIPERN03      =  7C +  9H +  6O +  N ; {@TLBIPERN03}       {}
TLEMUCN03       =  7C +  9H +  7O +  N ; {@TLEMUCN03}        {}
NCRES00H        =  7C +  9H +  8O +  N ; {@NCRES00H}         {}
MNCATEC00H      =  7C +  9H +  9O +  N ; {@MNCATEC00H}       {}
{8C (CH0)}
C8BC02          =  8C + 11H +  2O      ; {@C8BC02}           {MCM}
C721C03         =  8C + 11H +  5O      ; {@C721C03}          {MCM}
C8BCC0          =  8C + 12H +  0       ; {@C8BCC0}           {MCM}
C8BC00H         =  8C + 12H +  2O      ; {@C8BC00H}          {MCM}
C721CH0         =  8C + 12H +  3O      ; {@C721CH0}          {MCM}
N0RPINIC        =  8C + 12H +  4O      ; {@N0RPINIC}         {MCM}
C721C03H        =  8C + 12H +  5O      ; {@C721C03H}         {MCM}
C8502           =  8C + 13H +  3O      ; {@C8502}            {MCM}
C8902           =  8C + 13H +  3O      ; {@C8902}            {MCM}
C81102          =  8C + 13H +  4O      ; {@C81102}           {MCM}
C8602           =  8C + 13H +  4O      ; {@C8602}            {MCM}
C81202          =  8C + 13H +  5O      ; {@C81202}           {MCM}
C81302          =  8C + 13H +  5O      ; {@C81302}           {MCM}
C8BC            =  8C + 14H            ; {@C8BC}             {MCM}
C8500H          =  8C + 14H +  3O      ; {@C8500H}           {MCM}
C81100H         =  8C + 14H +  4O      ; {@C81100H}          {MCM}
C8600H          =  8C + 14H +  4O      ; {@C8600H}           {MCM}
C81200H         =  8C + 14H +  5O      ; {@C81200H}          {MCM}
C81300H         =  8C + 14H +  5O      ; {@C81300H}          {MCM}
C8900H          =  8C + 14H +  3O      ; {@C8900H}           {MCM}
C81O00H         =  8C + 14H +  4O      ; {@C81O00H}          {MCM}
C81O02          =  8C + 13H +  4O      ; {@C81O02}           {MCM}
{C8 (CH0) aromatics}
STYRENE         =  8C +  8H            ; {@STYRENE}          {styrene}
STYREN02        =  8C +  9H +  3O      ; {@STYREN02}         {}
LXYL            =  8C + 10H            ; {@LXYL}             {xylene}
EBENZ           =  8C + 10H            ; {@EBENZ}            {ethylbenzene}
STYREN00H       =  8C + 10H +  3O      ; {@STYREN00H}        {}
{8C (CH0N)}
C8BCN03         =  8C + 11H +  3O +  N ; {@C8BCN03}          {MCM}
C721PAN         =  8C + 11H +  7O +  N ; {@C721PAN}          {MCM}
C89N03          =  8C + 13H +  4O +  N ; {@C89N03}           {MCM}
C81ON03         =  8C + 14H +  5O +  N ; {@C81ON03}          {MCM}
{C8 (CH0N) aromatics}
NSTYREN02       =  8C +  8H +  5O +  N ; {@NSTYREN02}        {}
NSTYREN00H      =  8C +  9H +  5O +  N ; {@NSTYREN00H}       {}
{9C (CH0)}
C85C03          =  9C + 11H +  4O      ; {@C85C03}           {MCM}
N0PINDC0        =  9C + 12H +  2O      ; {@N0PINDC0}         {MCM}
C85C03H         =  9C + 12H +  4O      ; {@C85C03H}          {MCM}
N0PIND02        =  9C + 13H +  3O      ; {@N0PIND02}         {MCM}
C89C03          =  9C + 13H +  4O      ; {@C89C03}           {MCM}
C811C03         =  9C + 13H +  5O      ; {@C811C03}          {MCM}
N0PIN0NE        =  9C + 14H +  0       ; {@N0PIN0NE}         {MCM: nopinone}
N0PIN00         =  9C + 14H +  2O      ; {@N0PIN00}          {MCM}
N0RPINAL        =  9C + 14H +  2O      ; {@N0RPINAL}         {MCM: norpinaldehyde}
N0RPINEN0L      =  9C + 14H +  2O      ; {@N0RPINEN0L}       {norpinenol}
C89C02H         =  9C + 14H +  3O      ; {@C89C02H}          {MCM}
N0PIND00H       =  9C + 14H +  3O      ; {@N0PIND00H}        {MCM}
R06R3P          =  9C + 14H +  3O      ; {@R06R3P}           {from ref3019}
C89C03H         =  9C + 14H +  4O      ; {@C89C03H}          {MCM}
PINIC           =  9C + 14H +  4O      ; {@PINIC}            {MCM: pinic acid}
C811C03H        =  9C + 14H +  5O      ; {@C811C03H}         {MCM}
C96O2           =  9C + 15H +  3O      ; {@C96O2}            {MCM}
C9702           =  9C + 15H +  4O      ; {@C9702}            {MCM}
C9802           =  9C + 15H +  5O      ; {@C9802}            {MCM}
C96O0H          =  9C + 16H +  3O      ; {@C96O0H}           {MCM}
C9700H          =  9C + 16H +  4O      ; {@C9700H}           {MCM}
C9800H          =  9C + 16H +  5O      ; {@C9800H}           {MCM}
{9C (CH0N)}
C89PAN          =  9C + 13H +  5O +  N ; {@C89PAN}           {MCM}
C9PAN2          =  9C + 13H +  6O +  N ; {@C9PAN2}           {MCM}
C811PAN         =  9C + 13H +  7O +  N ; {@C811PAN}          {MCM}
C96N03          =  9C + 15H +  4O +  N ; {@C96N03}           {MCM}
C98N03          =  9C + 15H +  6O +  N ; {@C98N03}           {MCM}
{C9 aromatics (lumped)}
LTMB            =  9C + 12H            ; {@LTMB}             {trimethylbenzenes}
{10C (CH0)}
C10C9C0         = 10C + 10H +  3O      ; {@C10C9C0}          {MCM}
PINAL02         = 10C + 13H +  4O      ; {@PINAL02}          {MCM}
PINAL00H        = 10C + 14H +  4O      ; {@PINAL00H}         {MCM}
C10C902         = 10C + 15H +  4O      ; {@C10C902}          {MCM}
C96C03          = 10C + 15H +  4O      ; {@C96C03}           {MCM}
C10O602         = 10C + 15H +  5O      ; {@C10O602}          {MCM}
APINENE         = 10C + 16H            ; {@APINENE}          {MCM: alpha pinene}
BPINENE         = 10C + 16H            ; {@BPINENE}          {MCM: beta pinene}
CARENE          = 10C + 16H            ; {@CARENE}           {carene}
SABINENE        = 10C + 16H            ; {@SABINENE}         {sabinene}
CAMPHENE        = 10C + 16H            ; {@CAMPHENE}         {camphene}
PINAL           = 10C + 16H +  2O      ; {@PINAL}            {MCM: pinonaldehyde}
PINEN0L         = 10C + 16H +  2O      ; {@PINE0L}           {pinenol}
APINA00         = 10C + 16H +  3O      ; {@APINA00}          {stabilized APIN00A, not in MCM}
APINB00         = 10C + 16H +  3O      ; {@APINB00}          {MCM}
MENTHEN6ONE     = 10C + 16H +  3O      ; {@MENTHEN6ONE}      {8-00H-menthen-6-one, Taraborrelli,
pers. comm., not from MCM}
PIN0NIC         = 10C + 16H +  3O      ; {@PIN0NIC}          {MCM: pinonic acid}
C10C900H        = 10C + 16H +  4O      ; {@C10C900H}         {MCM}
PERPIN0NIC      = 10C + 16H +  4O      ; {@PERPIN0NIC}       {MCM}
C10O600H        = 10C + 16H +  5O      ; {@C10O600H}         {MCM}
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BPINA02         = 10C + 17H +  3O      ; {@BPINA02}          {MCM}
OH2MENTHEN6ONE  = 10C + 17H +  4O      ; {@2OHMENTHEN6ONE}   {2-OH-8-OOH-menthen-6-one,
Taraborrelli, pers. comm., not from MCM}
R06R102         = 10C + 17H +  4O      ; {@R06R102}          {cyclo-oxy peroxy radical from
BPINENE, ref3019}
R006R102        = 10C + 17H +  5O      ; {@R006R102}         {cyclo-peroxy peroxy radical from
BPINENE, ref3019}
R06R302         = 10C + 17H +  5O      ; {@R06R302}          {cyclo-oxy peroxy radical from
BPINENE, ref3019}
OHMENTHEN6ONE02 = 10C + 17H +  5O      ; {@OHMENTHEN6ONE02}  {2-OH-8-OOH_menthen-6-peroxy radical,
Taraborrelli, pers. comm., not from MCM}
BPINA00H        = 10C + 18H +  3O      ; {@BPINA00H}         {MCM}
R06R300H        = 10C + 18H +  5O      ; {@R06R300H}         {cyclo-oxy hydroperoxide from BPINENE,
ref3019}
{10C (CH0N)}
PINALN03        = 10C + 13H +  5O +  N ; {@PINALN03}         {MCM}
C10PAN2         = 10C + 15H +  6O +  N ; {@C10PAN2}          {MCM}
C106N03         = 10C + 15H +  6O +  N ; {@C106N03}          {MCM}
BPINAN03        = 10C + 17H +  4O +  N ; {@BPINAN03}         {MCM}
R06R1N03        = 10C + 17H +  5O +  N ; {@R06R1N03}         {nitrate from cyclo-oxy peroxy radical
from BPINENE, ref3019}
R06R3N03        = 10C + 17H +  6O +  N ; {@R06R3N03}         {nitrate from cyclo-oxy peroxy radical
from BPINENE, ref3019}
R006R1N03       = 10C + 17H +  6O +  N ; {@R006R1N03}        {nitrate from cyclo-peroxy peroxy
radical from BPINENE, ref3019}
{10C (lumped)}
LAPINAB02       = 10C + 17H +  3O      ; {@LAPINAB02}        {APINA02 and APINB02 lumped (ratio
1:2)}
LAPINAB00H      = 10C + 18H +  3O      ; {@LAPINAB00H}       {APINA00H and APINB00H lumped (ratio
1:2)}
LNAPINAB02      = 10C + 16H +  5O +  N ; {@LNAPINAB02}       {.65 NAPINA02 + .35 NAPINB02}
LNBPINAB02      = 10C + 16H +  5O +  N ; {@LNBPINAB02}       {.8 NBPINA02 + .2 NBPINB02}
LAPINABN03      = 10C + 17H +  4O +  N ; {@LAPINABN03}       {APINAN03 and APINBN03 lumped (ratio
1:2)}
LNAPINAB00H     = 10C + 17H +  5O +  N ; {@LNAPINAB00H}      {.65 NAPINA00H + .35 NAPINB00H}
LNBPINAB00H     = 10C + 17H +  5O +  N ; {@LNBPINAB00H}      {.8 NBPINA02 + .2 NBPINB02}
{C10 aromatics (lumped)}
LHAR0M          = 11C + 14H            ; {@LHAR0M}           {higher aromatics: model compound
DIET35T0L(from MCM)}
{---------------------------------- F ----------------------------------}
LFLU0RINE       = F                    ; {@LFLU0RINE}        {lumped F species}
{---------------------------------- Cl ---------------------------------}

Cl              = Cl                   ; {@Cl}               {chlorine atom}
Cl2             = 2Cl                  ; {@Cl_2}             {chlorine}
Cl0             = Cl + 0               ; {@Cl0}              {chlorine oxide}
HCl             = H + Cl               ; {@HCl}              {hydrochloric acid}
H0Cl            = H + 0 + Cl           ; {@H0Cl}             {hypochlorous acid}
Cl202           = 2Cl + 2O             ; {@Cl_2O_2}          {dichlorine dioxide}
0Cl0            = Cl + 2O              ; {@0Cl0}             {chlorine dioxide}
ClN02           = Cl + 2O + N          ; {@ClN0_2}           {nitryl chloride}
ClN03           = Cl + N + 3O          ; {@ClN0_3}           {chlorine nitrate}
CCl4            = C + 4Cl              ; {@CCl_4}            {tetrachloro methane}
CH3Cl           = C + 3H + Cl          ; {@CH_3Cl}           {chloromethane}
CH3CCl3         = 2C + 3H + 3Cl        ; {@CH_3CCl_3}        {1,1,1-trichloroethane = methyl
chloroform = MCF}
CF2Cl2          = C + 2F + 2Cl         ; {@CF_2Cl_2}         {dichlorodifluoromethane = F12}
CFCl3           = C + F + 3Cl          ; {@CFCl_3}           {trichlorofluoromethane = F11}
LCHL0RINE       = Cl                   ; {@LCHL0RINE}        {lumped Cl species}

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

Br              = Br                   ; {@Br}               {bromine atom}
Br2             = 2Br                  ; {@Br_2}             {bromine}
Br0             = Br + 0               ; {@Br0}              {bromine oxide}
HBr             = H + Br               ; {@HBr}              {hydrobromic acid}
H0Br            = H + 0 + Br           ; {@H0Br}             {hypobromous acid}
BrN02           = Br + N + 2O          ; {@BrN0_2}           {nitryl bromide}
BrN03           = Br + N + 3O          ; {@BrN0_3}           {bromine nitrate}
BrCl            = Br + Cl              ; {@BrCl}             {bromine chloride}
CH3Br           = Br + C +3H           ; {@CH_3Br}           {bromomethane}
CF3Br           = Br + 3F + C          ; {@CF_3Br}           {Halon 1301}
CF2ClBr         = Br + 2F + Cl + C     ; {@CF_2ClBr}         {Halon 1211}
CHCl2Br         = C + H + 2Cl + Br     ; {@CHCl_2Br}         {}
CHClBr2         = C + H + Cl + 2Br     ; {@CHClBr_2}         {}
CH2ClBr         = C + 2H + Cl + Br     ; {@CH_2ClBr}         {}
CH2Br2          = C + 2H + 2Br         ; {@CH_2Br_2}         {}
CHBr3           = C + H + 3Br          ; {@CHBr_3}           {}
LBR0MINE        = Br                   ; {@LBR0MINE}         {lumped Br species}

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

I               = I                    ; {@I}                {iodine atomic ground state}
I2              = 2I                   ; {@I_2}              {molecular iodine}
I0              = I + 0                ; {@I0}               {iodine monoxide radical}
0I0             = I + 2O               ; {@0I0}              {}
I202            = 2O + 2I              ; {@I_2O_2}           {}
HI              = H + I                ; {@HI}               {hydrogen iodide}
H0I             = H + 0 + I            ; {@H0I}              {hypoiodous acid}
HI03            = H + I + 3O           ; {@HI0_3}            {}
IN02            = I + N + 2O           ; {@IN0_2}            {iodine nitrite}
IN03            = I + N + 3O           ; {@IN0_3}            {iodine nitrate}
CH3I            = C + 3H + I           ; {@CH_3I}            {iodomethane}
CH2I2           = C + 2H + 2I          ; {@CH_2I_2}          {diiodomethane}
C3H7I           = 3C + 7H + I          ; {@CH_3CHICH_3}      {2-iodopropane}
ICl             = I + Cl               ; {@ICl}              {iodine chloride}
CH2ClI          = C + 2H + Cl + I      ; {@CH_2ClI}          {chloroiodomethane}
IBr             = I + Br               ; {@IBr}              {iodine bromide}
IPART           = 2I                   ; {@I(part)}          {iodine particles}

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

S               = S                    ; {@S}                {sulfur atomic ground state}
S0              = S + 0                ; {@S0}               {sulfur monoxide}
S02             = S + 2O               ; {@S0_2}             {sulfur dioxide}
S03             = S + 3O               ; {@S0_3}             {sulfur trioxide}
SH              = S + H                ; {@SH}               {}
H2S04           = 2H + S + 4O          ; {@H_2S0_4}          {sulfuric acid}
CH3S03H         = C + 4H + S + 3O      ; {@CH_3S0_3H}        {MSA: methane sulfonic acid}
DMS             = 2C + 6H + S          ; {@DMS}              {dimethyl sulfide}
DMS0            = 2C + 6H + S + 0      ; {@DMS0}             {dimethyl sulfoxide: CH3S0CH3}
CH3S02          = C + 3H + S + 2O      ; {@CH_3S0_2}         {}
CH3S03          = C + 3H + S + 3O      ; {@CH_3S0_3}         {}
0CS             = C + S + 0            ; {@0CS}              {}
LSULFUR         = S                    ; {@LSULFUR}          {lumped S species}

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

Hg              = Hg                   ; {@Hg}               {}
Hg0             = Hg + 0               ; {@Hg0}              {}
HgCl            = Hg + Cl              ; {@HgCl}             {}
HgCl2           = Hg + 2Cl             ; {@HgCl_2}           {}
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```
HgBr            = Hg + Br               ; {@HgBr}             {}
HgBr2           = Hg + 2Br              ; {@HgBr_2}           {}
ClHgBr          = Hg + Cl + Br          ; {@ClHgBr}           {}
BrHg0Br         = Hg + O + 2Br          ; {@BrHg0Br}          {}
ClHg0Br         = Hg + O + Cl + Br      ; {@ClHg0Br}          {}

{--- mz_pj_20070209+}
{------------------------ Pseudo Aerosol ----------------------------------}
N03m_cs         = N + 3O                ; {@NO_3^-\aq}        {}
Hp_cs           = H                     ; {@H^+\aq}           {}
RGM_cs          = Hg                    ; {@Hg\aq}            {from reactive gaseous Hg}
{--- mz_pj_20070209-}

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

Dummy           = Ignore                ; {@Dummy}            {just a dummy}

{ mz_pj_20070621+}
{------------------------ O3 Budget Tracers (via eval2.3.rpl) -------------}
O3s             = 3O                    ; {@O_3(s)}           {strat. ozone}
L03s            = Ignore                ; {@LO_3(s)}          {lost strat. ozone}
{ mz_pj_20070621-}

{ mz_rs_20100227+}
{only for MIM1, not used in MIM2:}
LHOC3H602       = 3C + 7H + 3O          ; {@CH_3CH(O_2)CH_2OH} {hydroxyperoxyradical from propene+OH}
LHOC3H600H      = 3C + 8H + 3O          ; {@CH_3CH(OOH)CH_2OH} {C3H6OHOOH = hydroxyhydroperoxides
from C3H6}
IS02            = 5C + 9H + 3O          ; {@IS02}             {isoprene (hydroxy) peroxy radicals}
IS0N            = 5C +           N      ; {@IS0N}             {organic nitrates from IS02 and
C5H8+NO3}
IS00H           = 5C + 10H + 3O         ; {@IS00H}            {isoprene (hydro) peroxides}
MVK02           = 4C + 7H + 4O          ; {@MVK02}            {MVK/MACR peroxy radicals}
MVK00H          = 4C + 8H + 4O          ; {@MVK00H}           {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 ------------------}
CFC13_c         = C + F + 3Cl           ; {@(CFCl_3)_c}       {trichlorofluoromethane = F11}
CF2C12_c        = C + 2F + 2Cl          ; {@(CF_2Cl_2)_c}     {dichlorodifluoromethane = F12}
N20_c           = O + 2N                ; {@(N_2O)_c}         {nitrous oxide}
CH3CC13_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}
LAR01           =  Ignore               ; {@LAR01}            {aromatic VOC}
LAR02           =  Ignore               ; {@LAR02}            {aromatic VOC}
LOLE1           =  Ignore               ; {@LOLE1}            {olefins}
LOLE2           =  Ignore               ; {@LOLE2}            {olefins}
LfPOGO2         =  Ignore               ; {@LfPOGO2}          {FF  condensable gas 2}
LfPOGO3         =  Ignore               ; {@LfPOGO3}          {FF  condensable gas 3}
LfPOGO4         =  Ignore               ; {@LfPOGO4}          {FF  condensable gas 4}
LbbPOGO2        =  Ignore               ; {@LbbPOGO2}         {BB  condensable gas 2}
LbbPOGO3        =  Ignore               ; {@LbbPOGO3}         {BB  condensable gas 3}
LbbPOGO4        =  Ignore               ; {@LbbPOGO4}         {BB  condensable gas 4}
LfSOGsv01       =  Ignore               ; {@LfSOGsv01}        {sFF condensable gas 1}
LbbSOGsv01      =  Ignore               ; {@LbbSOGsv01}       {sBB condensable gas 1}
LfSOGiv01       =  Ignore               ; {@LfSOGiv01}        {iFF condensable gas 1}
LfSOGiv02       =  Ignore               ; {@LfSOGiv02}        {iFF condensable gas 2}
LfSOGiv03       =  Ignore               ; {@LfSOGiv03}        {iFF condensable gas 3}
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}
Lb0SOGv01       =  Ignore               ; {@Lb0SOGv01}        {Bio condensable gas 1}
Lb0SOGv02       =  Ignore               ; {@Lb0SOGv02}        {Bio condensable gas 2}
Lb0SOGv03       =  Ignore               ; {@Lb0SOGv03}        {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}
La0SOGv01       =  Ignore               ; {@La0SOGv01}        {Ant condensable gas 1}
La0SOGv02       =  Ignore               ; {@La0SOGv02}        {Ant condensable gas 2}
La0SOGv03       =  Ignore               ; {@La0SOGv03}        {Ant condensable gas 3}
{ mz_at_20131015- needed for ORACLE.rpl}
{***** END:   gas-phase species from gas_mom-4pub.spc *****}
{**** START: aerosol species (phase 1) from aqueous.spc ****}
{------------------------------------------------------------------------}
{----------------------------- aerosol mode: 01# --------------------------}
{------------------------------------------------------------------------}

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

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

 O2_a01         = IGNORE; {@O_2\aq}          {oxygen}
 O3_a01         = IGNORE; {@O_3\aq}          {ozone}

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

 OH_a01         = IGNORE; {@OH\aq}           {hydroxyl radical}
 HO2_a01        = IGNORE; {@HO_2\aq}         {perhydroxyl radical}
 H2O_a01        = IGNORE; {@H_2O\aq}         {water}
 H2O2_a01       = IGNORE; {@H_2O_2\aq}       {hydrogen peroxide}

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

 NH3_a01        = IGNORE; {@NH_3\aq}         {ammonia}
 NO_a01         = IGNORE; {@NO\aq}           {nitric oxide}
 NO2_a01        = IGNORE; {@NO_2\aq}         {nitrogen dioxide}
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 NO3_aq      = IGNORE; {@NO_3\aq}        {nitrogen trioxide}
 HONO_aq     = IGNORE; {@HONO\aq}        {nitrous acid}
 HNO3_aq     = IGNORE; {@HNO_3\aq}       {nitric acid}
 HNO4_aq     = IGNORE; {@HNO_4\aq}       {pernitric acid}
 N2O5_aq     = IGNORE; {@N_2O_5\aq}      {dinitrogen pentoxide}

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

{1C}
 CH3OH_aq    = IGNORE; {@CH_3OH\aq}      {methanol}
 HCOOH_aq    = IGNORE; {@HCOOH\aq}       {formic acid}
 HCHO_aq     = IGNORE; {@HCHO\aq}        {methanal (formaldehyde)}
 CH3O2_aq    = IGNORE; {@CH_3O2\aq}      {methylperoxy radical}
 CH3OOH_aq   = IGNORE; {@CH_3OOH\aq}     {}
 CO2_aq      = IGNORE; {@CO_2\aq}        {carbon dioxide}

{2C}
 CH3CO2H_aq  = IGNORE; {@CH_3COOH\aq}    {acetic acid}
 PAN_aq      = IGNORE; {@PAN\aq}         {peroxyacetylnitrate}
 C2H5O2_aq   = IGNORE; {@C_2H_5O_2\aq}   {ethylperoxy radical}
 CH3CHO_aq   = IGNORE; {@CH_3CHO\aq}     {acetaldehyde}

{3C}
 CH3COCH3_aq = IGNORE; {@CH_3COCH_3\aq}  {acetone}

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

 Cl_aq       = IGNORE; {@Cl\aq}          {chlorine atom}
 Cl2_aq      = IGNORE; {@Cl_2\aq}        {molecular chlorine}
 HCl_aq      = IGNORE; {@HCl\aq}         {hydrogen chloride}
 HOCl_aq     = IGNORE; {@HOCl\aq}        {hypochlorous acid}

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

 Br_aq       = IGNORE; {@Br\aq}          {bromine atom}
 Br2_aq      = IGNORE; {@Br_2\aq}        {molecular bromine}
 HBr_aq      = IGNORE; {@HBr\aq}         {hydrogen bromide}
 HOBr_aq     = IGNORE; {@HOBr\aq}        {hypobromous acid}
 BrCl_aq     = IGNORE; {@BrCl\aq}        {bromine chloride}

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

 I2_aq       = IGNORE; {@I_2\aq}         {molecular iodine}
 IO_aq       = IGNORE; {@IO\aq}          {iodine monoxide radical}
 HI_aq       = IGNORE; {@HI\aq}          {hydrogen iodide}
 HOI_aq      = IGNORE; {@HOI\aq}         {hypoiodous acid}
 ICl_aq      = IGNORE; {@ICl\aq}         {iodine chloride}
 IBr_aq      = IGNORE; {@IBr\aq}         {iodine bromide}
 HIO3_aq     = IGNORE; {@HIO_3\aq}       {iodic acid}

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

 SO2_aq      = IGNORE; {@SO_2\aq}        {sulfur dioxide}
 H2SO4_aq    = IGNORE; {@H_2SO_4\aq}     {sulfuric acid}
 DMS_aq      = IGNORE; {@DMS\aq}         {dimethyl sulfide: CH3SCH3}
 DMSO_aq     = IGNORE; {@DMSO\aq}        {dimethyl sulfoxide: CH3SOCH3}

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

 Hg_aq       = IGNORE; {@Hg\aq}          {mercury}
 HgO_aq      = IGNORE; {@HgO\aq}         {}
 HgOH_aq     = IGNORE; {@HgOH\aq}        {}
 HgOHOH_aq   = IGNORE; {@Hg(OH)_2\aq}    {}
 HgOHCl_aq   = IGNORE; {@Hg(OH)Cl\aq}    {}
 HgCl2_aq    = IGNORE; {@HgCl_2\aq}      {}
 HgBr2_aq    = IGNORE; {@HgBr_2\aq}      {}
 HgSO3_aq    = IGNORE; {@HgSO_3\aq}      {}
 ClHgBr_aq   = IGNORE; {@ClHgBr\aq}      {}
 BrHgOBr_aq  = IGNORE; {@BrHgOBr\aq}     {}
 ClHgOBr_aq  = IGNORE; {@ClHgOBr\aq}     {}

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

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

 O2m_aq      = IGNORE; {@O_2^-\aq}       {}
 OHm_aq      = IGNORE; {@OH^-\aq}        {}

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

 Hp_aq       = IGNORE; {@H^+\aq}         {}

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

 NH4p_aq     = IGNORE; {@NH_4^+\aq}      {ammonium}
 NO2m_aq     = IGNORE; {@NO_2^-\aq}      {nitrite}
 NO3m_aq     = IGNORE; {@NO_3^-\aq}      {nitrate}
 NO4m_aq     = IGNORE; {@NO_4^-\aq}      {peroxy nitrate}

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

{1C}
 CO3m_aq     = IGNORE; {@CO_3^-\aq}      {}
 HCOOm_aq    = IGNORE; {@HCOO^-\aq}      {formate}
 HCO3m_aq    = IGNORE; {@HCO_3^-\aq}     {hydrogen carbonate}

{2C}
 CH3COOm_aq  = IGNORE; {@CH_3COO^-\aq}   {acetate}

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

 Clm_aq      = IGNORE; {@Cl^-\aq}        {chloride}
 Cl2m_aq     = IGNORE; {@Cl_2^-\aq}      {}
 ClOm_aq     = IGNORE; {@ClO^-\aq}       {}
 ClOHm_aq    = IGNORE; {@ClOH^-\aq}      {}

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

 Brm_aq      = IGNORE; {@Br^-\aq}        {bromide}
 Br2m_aq     = IGNORE; {@Br_2^-\aq}      {}
 BrOm_aq     = IGNORE; {@BrO^-\aq}       {}
 BrOHm_aq    = IGNORE; {@BrOH^-\aq}      {}
 BrCl2m_aq   = IGNORE; {@BrCl_2^-\aq}    {}
 Br2Clm_aq   = IGNORE; {@Br_2Cl^-\aq}    {}

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

 Im_aq       = IGNORE; {@I^-\aq}         {iodide}
 IO2m_aq     = IGNORE; {@IO_2^-\aq}      {}
 IO3m_aq     = IGNORE; {@IO_3^-\aq}      {iodate}
 ICl2m_aq    = IGNORE; {@ICl_2^-\aq}     {}
 IClBrm_aq   = IGNORE; {@IClBr^-\aq}     {}
```

```
 IBr2m_aQ1      = IGNORE; {@IBr_2^-\aq}      {}

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

 SO3m_aQ1       = IGNORE; {@SO_3^-\aq}       {}
 SO3mm_aQ1      = IGNORE; {@SO_3^<2->\aq}    {sulfite}
 SO4m_aQ1       = IGNORE; {@SO_4^-\aq}       {}
 SO4mm_aQ1      = IGNORE; {@SO_4^<2->\aq}    {sulfate}
 SO5m_aQ1       = IGNORE; {@SO_5^-\aq}       {}
 HSO3m_aQ1      = IGNORE; {@HSO_3^-\aq}      {hydrogen sulfite}
 HSO4m_aQ1      = IGNORE; {@HSO_4^-\aq}      {hydrogen sulfate}
 HSO5m_aQ1      = IGNORE; {@HSO_5^-\aq}      {}
 CH3SO3m_aQ1    = IGNORE; {@CH_3SO_3^-\aq}   {MSA anion}
 CH2OHSO3m_aQ1  = IGNORE; {@CH_2OHSO_3^-\aq} {}

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

 Hgp_aQ1        = IGNORE; {@Hg^+\aq}             {}
 Hgpp_aQ1       = IGNORE; {@Hg^<2+>\aq}          {}
 HgOHp_aQ1      = IGNORE; {@HgOH^+\aq}           {}
 HgClp_aQ1      = IGNORE; {@HgCl^+\aq}           {}
 HgCl3m_aQ1     = IGNORE; {@HgCl_3^-\aq}         {}
 HgCl4mm_aQ1    = IGNORE; {@HgCl_4^<2->\aq}      {}
 HgBrp_aQ1      = IGNORE; {@HgBr^+\aq}           {}
 HgBr3m_aQ1     = IGNORE; {@HgBr_3^-\aq}         {}
 HgBr4mm_aQ1    = IGNORE; {@HgBr_4^<2->\aq}      {}
 HgSO32mm_aQ1   = IGNORE; {@Hg(SO_3)_2^<2->\aq}  {}

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

 DUMMY_aQ1      = IGNORE; {@DUMMY\aq}        {}
 DUM2_aQ1       = IGNORE; {@DUM2\aq}         {}
 DUMH_aQ1       = IGNORE; {@DUMH^+\aq}       {}
 DUMA_aQ1       = IGNORE; {@DUMA\aq}         {}
 DUMAm_aQ1      = IGNORE; {@DUMA^-\aq}       {}
 DUMGtAi_aQ1    = IGNORE; {@DUMGtAi\aq}      {}
 DUMGtAs_aQ1    = IGNORE; {@DUMGtAs\aq}      {}
 PRODUM1_aQ1    = IGNORE; {@PRODUM1\aq}      {}
 PRODUM2_aQ1    = IGNORE; {@PRODUM2\aq}      {}
 Nap_aQ1        = IGNORE; {@Na^+\aq}         {dummy cation}
{**** END:   aerosol species (phase 1) from aqueous.spc ****}
{SETFIX H2O_a* is done via xmecca}
```

```
{This file was created automatically by xmecca, DO NOT EDIT!}
#INLINE F90_GLOBAL
  ! MECCA info from xmecca:
  CHARACTER(LEN=*), PUBLIC, PARAMETER :: &
    timestamp = 'xmecca was run on 2015-11-14 at 19:50:16 by sgromov on machine hydra05', &
    gas_spc_file         = '-rw------- 1 sgromov mpc 63625 Nov 14 17:48 gas_mom.spc', &
    aqueous_spc_file     = '-rw-rw---- 1 sgromov mpc 8444 Apr 19  2010 aqueous.spc', &
    gas_eqn_file         = '-rw------- 1 sgromov mpc 320486 Nov 14 11:20 gas_mom.eqn', &
    aqueous_eqn_file     = '-rw-rw---- 1 sgromov mpc 56776 Jul 13  2010 aqueous.eqn', &
    gas_spc_file_sum     = '24076    63', &
    aqueous_spc_file_sum = '54945     9', &
    gas_eqn_file_sum     = '29603   313', &
    aqueous_eqn_file_sum = '12944    56', &
    rplfile              = 'COS', &
    wanted               = '(((Tr && (G || Het) && !I) || St) && !Hg)', &
    diagtracfile         = '', &
    rxnrates             = 'n', &
    tagdbl               = 'n'
  LOGICAL, PARAMETER :: REQ_MCFCT = .FALSE.
#ENDINLINE {above lines go to messy_mecca_kpp_global}
#INLINE F90_GLOBAL
  ! from xmecca for aerosol:
  INTEGER, PARAMETER, PUBLIC :: APN = 1
  ! from aerosol.awk:
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_O2_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_O3_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_OH_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HO2_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_H2O_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_H2O2_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NH3_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NO_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NO2_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NO3_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HONO_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HNO3_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HNO4_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_N2O5_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3OH_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HCOOH_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HCHO_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3O2_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3OOH_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CO2_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3CO2H_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_PAN_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_C2H5O2_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3CHO_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3COCH3_a  = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Cl_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Cl2_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HCl_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HOCl_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Br_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Br2_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HBr_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HOBr_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_BrCl_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_I2_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_IO_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HI_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HOI_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_ICl_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_IBr_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HIO3_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_SO2_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_H2SO4_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DMS_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DMSO_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hg_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hg0_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hg0H_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hg0H0H_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hg0HCl_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgCl2_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgBr2_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgSO3_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_ClHgBr_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_BrHg0Br_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_ClHg0Br_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_O2m_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_OHm_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hp_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NH4p_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NO2m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NO3m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_NO4m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CO3m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HCOOm_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HCO3m_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3COOm_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Clm_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Cl2m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_ClOm_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_ClOHm_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Brm_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Br2m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_BrOm_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_BrOHm_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_BrCl2m_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Br2Clm_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Im_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_IO2m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_IO3m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_ICl2m_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_IClBrm_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_IBr2m_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_SO3m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_SO3mm_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_SO4m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_SO4mm_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_SO5m_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HSO3m_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HSO4m_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HSO5m_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH3SO3m_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_CH2OHSO3m_a = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hgp_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hgpp_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Hg0Hp_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgClp_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgCl3m_a    = 0
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```
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgCl4mm_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgBrp_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgBr3m_a    = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgBr4mm_a   = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_HgSO32mm_a  = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DL0_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_D20_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DAHp_a      = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DA_a        = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DAm_a       = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DGtAi_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_DGtAs_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_PRODL_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_PROD2_a     = 0
  INTEGER, PUBLIC, DIMENSION(APN) :: ind_Nap_a       = 0
#ENDINLINE {above lines go to messy_mecca_kpp_global}
#INLINE F90_UTIL
! from xmecca:
SUBROUTINE initialize_indexarrays
  USE messy_mecca_kpp_global     ! ind_XYZ_a(:) arrays
  USE messy_mecca_kpp_parameters ! ind_XYZ_a## scalars
  IMPLICIT NONE
END SUBROUTINE initialize_indexarrays
#ENDINLINE {above lines go to messy_mecca_kpp_util}
{***** START: gas-phase chemistry from gas_mom.eqn *****}
#INLINE F90_GLOBAL
  ! variable declarations from gas.eqn:
  ! ------------------------------------------------------------------------
  ! inorganic and Cl chemistry:
  REAL :: k_HO2_HO2, k_NO3_NO2, k_NO2_HO2, k_HNO3_OH, k_CH3OOH_OH, &
          k_ClO_ClO, k_BrO_NO2, k_I_NO2, k_DMS_OH, k_CH2OO_SO2
  REAL :: k_O3s ! used in some *.rpl files
  ! new methane chemistry:
  REAL :: beta_null_CH3NO3, beta_inf_CH3NO3, beta_CH3NO3, &
          k_NO2_CH3O2, k_CH2OO_NO2, beta_C2H5NO3, k_C6H5O2_NO2
  ! ------------------------------------------------------------------------
  ! only for mim1, see mim1.rpl:
  REAL :: k_Pr02_HO2, k_Pr02_NO, k_Pr02_CH3O2
  REAL :: kO_NO_HO2, k1d_NO_HO2, k1w_NO_HO2, k2d_NO_HO2, k2w_NO_HO2, &
          alpha_NO_HO2, beta_NO_HO2, G740a_yield
  ! end of mim1 block
  ! ------------------------------------------------------------------------
  ! organic chemistry (MIM, MAM, MOM...):
  REAL :: k_CH3CO3_NO2, k_PAN_M
  REAL(dp) :: KRO2NO, KAPHO2, KAPNO, KRO2NO3, KNO3AL
  ! maximum no. of C atoms the rate coefficients are calculated for:
  INTEGER,  PARAMETER :: MAXnC = 12
  INTEGER :: nCi ! nC index runner
  ! carbon nos. to calculate the lookup table for RO2+HO2 rate coeffs., etc.:
  INTEGER,  PARAMETER :: nC(MAXnC) = (/ (nCi,nCi=1,MAXnC) /)
  REAL(dp) :: KRO2HO2(MAXnC)
  REAL :: KHSB, KHSD, K16HS, K16HSZ14, K16HSZ41, K15HSDHB, K14HSAL, &
          K15HS24VYNAL, K15HS42VYNAL, KHYDEC
  REAL :: J_IC3H7NO3, J_ACETOL, J_HPALD, J_KETENE
  REAL(dp) :: RO2      ! sum of peroxy radicals
  REAL(dp) :: k_CH3O2   ! CH3O2 self-reaction
  REAL(dp) :: k_RO2RCO3, k_RO2pRO2, k_RO2sRO2, k_RO2tRO2, &
              k_RO2pORO2, k_RO2sORO2, k_RO2tORO2, &
              k_RO2LISOPACO2, k_RO2ISOPBO2, k_RO2ISOPDO2
  REAL(dp) :: k_CH2CH0H_OH_HCOOH, k_CH2CH0H_OH_ALD, k_CH2CH0H_HCOOH, k_ALD_HCOOH
  REAL(dp) :: k1_RO2RCO3, k1_RO2pRO2, k1_RO2sRO2, k1_RO2tRO2, &
              k1_RO2pORO2, k1_RO2sORO2, k1_RO2tORO2, &
              k1_RO2LISOPACO2, k1_RO2ISOPBO2, k1_RO2ISOPDO2
  REAL(dp), PARAMETER :: k_C6H5O_NO2  = 2.08E-12 ! ref3172
  REAL(dp), PARAMETER :: k_C6H5O_O3   = 2.86E-13 ! ref3171
  ! SAR for OH reactions (ref3030 with introduction of temperature dependency)
  ! parameters for the SAR on H-abstraction OH:
  REAL(dp) :: k_p, k_s, k_t, k_rohro, k_co2h
  REAL(dp), PARAMETER :: &
    f_soh = 3.44, f_toh = 2.68, &
    f_sooh = 7.,  f_tooh = 7., & ! from Wang and Chen, ref3196
    f_ono2 = 0.04 , f_ch2ono2 = 0.2, &
    f_cpan= .25, f_allyl = 3.6, f_alk= 1.23, &
    f_cho = 0.55, f_co2h = 1.67, f_co = 0.73, &
    f_o = 8.15, f_pch2oh = 1.29, f_tch2oh = 0.53
  ! parameters for the SAR on OH-addtion to alkenes
  ! Note for ach2ooh calculated
  ! assuming RO2 distribution in ref3159
  ! B, E, D, F, AC are .41, .02, .22, .05, .30 respectively
  REAL(dp) :: k_adp, k_ads, k_adt
  REAL(dp), PARAMETER :: &
    k_adsecprim = 3.0E-11, k_adtertprim = 5.7E-11, &
   , a_pan = 0.56      , a_cho = 0.31   , a_coch3 = 0.76, &
   , a_ch2ono2 = 0.64  , a_ch2oh = 1.7  , a_ch2ooh = 1.7, &
   , a_coh = 2.2       , a_cooh = 2.2   , a_co2h = 0.25
  REAL(dp), PARAMETER :: KDEC = 1.E6
  ! Branching ratios for RO2 + HO2 reactions
  ! CH3CO3 + HO2 has unique branching ratios (see reaction)
  ! beta-hydroxy acyl peroxy radicals, e.g. HOCH2CO3
  ! (GroÃŸ, PhD Thesis, ref3195)
  REAL(dp), PARAMETER :: rco3_oh  = 0.69, rco3_o3  = 0.10, rco3_ooh = 0.21
  ! beta-keto peroxy radicals equal or bigger than CH3COCH2O2CH3 (Dillon and Crowley, ref3192)
  REAL(dp), PARAMETER :: rcoch2o2_oh  = 0.15, rcoch2o2_ooh = 0.85
  REAL(dp), PARAMETER :: rchohch2o2_oh = 0.10 ! derived from Liu ref3193 for ISOPBO2 and ISOPDO2.
Consistent with exp. data by C. GroÃŸ (MPIC)
  REAL(dp), PARAMETER :: rch2och2o2_oh  = 0.4 ! ref3175 for CH3OCH2O2
  REAL(dp), PARAMETER :: rbipero2_oh = 0.40 ! ref3188 for toluene
  REAL(dp), PARAMETER :: fhpal = 0.5 ! HPALD-yield after 1,6-H-shift
  ! ------------------------------------------------------------------------
!KPPPP_DIRECTIVE vector variable definition start
  ! IMPORTANT NOTES ABOUT TEMP, PRESS, AND CAIR:
  ! - The KPP variable "temp" is already defined automatically by KPP in
  !   messy_mecca_kpp_global.f90. The KPP variables "press" and "cair" are
  !   defined here.
  ! - The 3 variables temp, press, and cair are only used inside KPP.
  !   They are different from the variables with the same names in the base
  !   model (as used in the SMIL files *_si.f90 and *_box.f90)
  ! - Data transfer between the SMIL and the KPP variables is done via the
  !   fill subroutines in messy_mecca_kpp.f90:
  !   - fill_temp transfers temperature
  !   - fill_press transfers pressure
  !   - fill_cair transfers cair (this is redundant because cair could be
  !     calculated from temp and press; nevertheless, redundant transfer to
  !     KPP is preferred to avoid potential numerical differences when
  !     recalculating cair inside KPP)
  REAL(dp) :: cair      ! c(air) (wet) [mcl/cm^3]
  REAL(dp) :: press     ! pressure [Pa]
  REAL(dp) :: temp_ion  ! ion temperature [K]
  REAL(dp) :: temp_elec ! electron temperature [K]
!KPPPP_DIRECTIVE vector variable definition end
  ! AEROSOL ONLY:
!KPPPP_DIRECTIVE vector variable definition start
```

```
  REAL(dp) :: xaer(APN)
  REAL(dp) :: cvfac(APN)    ! unit conversion factor
  REAL(dp) :: lwc(APN)      ! liquid water content
  REAL(dp) :: k_exf(APN,NSPEC) = 0.
  REAL(dp) :: k_exb(APN,NSPEC) = 0.
  REAL(dp) :: k_exf_N2O5(APN)  = 0.
  REAL(dp) :: k_exf_ClNO3(APN) = 0.
  REAL(dp) :: k_exf_BrNO3(APN) = 0.
!KPPPP_DIRECTIVE vector variable definition end
  INTEGER, PUBLIC  :: xnom7sulf = 1 ! = 1-xm7sulf
!KPPPP_DIRECTIVE vector variable definition start
  REAL(dp) :: jx(IP_MAX) = 0.
!KPPPP_DIRECTIVE vector variable definition end
  ! iht_ = index of troposheric heterogeneous reactions
  INTEGER, PARAMETER, PUBLIC :: &
    iht_N2O5      =  1, iht_HNO3      =  2, iht_Hg      =  3, &
    iht_RGM       = 4
  INTEGER, PARAMETER, PUBLIC :: IHT_MAX = 4
!KPPPP_DIRECTIVE vector variable definition start
  REAL(dp) :: khet_Tr(IHT_MAX) = 0.
!KPPPP_DIRECTIVE vector variable definition end
  ! ihs_ = index of stratospheric heterogeneous reactions
  ! (must be the same as in messy_msbm.f90!)
  INTEGER, PARAMETER :: &
    ihs_N2O5_H2O  =  1, ihs_HOCl_HCl  =  2, ihs_ClNO3_HCl =  3, &
    ihs_ClNO3_H2O =  4, ihs_N2O5_HCl  =  5, ihs_ClNO3_HBr =  6, &
    ihs_BrNO3_HCl =  7, ihs_HOCl_HBr  =  8, ihs_HOBr_HCl  =  9, &
    ihs_HOBr_HBr  = 10, ihs_BrNO3_H2O = 11, ihs_Hg        = 12, &
    ihs_RGM       = 13
  INTEGER, PARAMETER, PUBLIC :: IHS_MAX = 13
!KPPPP_DIRECTIVE vector variable definition start
  REAL(dp) :: khet_St(IHS_MAX) = 0.
!KPPPP_DIRECTIVE vector variable definition end
  ! Parameters included for acid-base equilibria calculation
  ! used to enable the double use of the aqueous.eqn for liquid
  ! and aerosol phase.
  REAL(dp), PARAMETER :: &
    testfac_H2O   = 1.e5_dp, testfac_HONO   = 1.e5_dp, &
    testfac_HNO3  = 1.e7_dp, testfac_HNO4   = 1.e5_dp, &
    testfac_HCOOH = 1.e5_dp, testfac_SO2    = 1.e9_dp, &
    testfac_HSO3m = 1.e9_dp, testfac_HSO4m  = 1.e7_dp, &
    testfac_NH3   = 1.e7_dp, testfac_H2O    = 1.e9_dp, &
    testfac_CO2   = 1.e5_dp, testfac_HCl    = 1.e2_dp, &
    testfac_HBr   = 1.e6_dp,                           &
    testfac_HOCl  = 1.e2_dp, testfac_HOBr   = 1.e2_dp, &
    testfac_ICl   = 1.e2_dp, testfac_IBr    = 1.e2_dp, &
    testfac_IClBr = 1.e2_dp, testfac_H2SO4  = 1.e7_dp
#ENDINLINE {above lines go to messy_mecca_kpp_global}
#INLINE F90_INIT
  rtol(:) = 1E-2_dp ! relative tolerance
  atol(:) = 1E1_dp  ! absolute tolerance
  IF ((ind_OH  >0).AND.(ind_OH  <=NVAR)) atol(ind_OH)  = 1._dp
  IF ((ind_NO3 >0).AND.(ind_NO3 <=NVAR)) atol(ind_NO3) = 1._dp
  IF ((ind_Cl  >0).AND.(ind_Cl  <=NVAR)) atol(ind_Cl)  = 1._dp
  IF ((ind_Br  >0).AND.(ind_Br  <=NVAR)) atol(ind_Br)  = 1._dp
  IF ((ind_O1D >0).AND.(ind_O1D <=NVAR)) atol(ind_O1D) = 1._dp
#ENDINLINE {above lines go to the end of subroutine Initialize}
#INLINE F90_RCONST
  USE messy_main_constants_mem ! atm2Pa, N_A, R_gas
  USE messy_cmn_photol_mem     ! IP_MAX, ip_*, jname
  ! end of USE statements
  !
  ! start of executable statements
  ! define some rate constants here if the expressions are too long
  ! for kpp or if they are used more than once
  ! ------------------------------------------------------------------------
  ! inorganic and Cl chemistry:
  k_HO2_HO2    = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* & ! {1.5+/-0.2}
                 (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))
  k_NO3_NO2    = k_3rd(temp,cair,2.0E-30,4.4,1.4E-12,0.7,0.6)
  k_NO2_HO2    = k_3rd(temp,cair,2.0E-31,3.4,2.9E-12,1.1,0.6)
  k_HNO3_OH    = 2.4E-14*EXP(460./temp) + 1./ &
                 ( 1./(6.5E-34*EXP(1335./temp)*cair) + &
                 1./(2.7E-17*EXP(2199./temp)) )
  k_CH3OOH_OH  = 5.3E-12*EXP(190./temp)
  k_ClO_ClO    = k_3rd_iupac(temp,cair,2.0E-32, &
                 4.0,1.0E-11,0.0,0.45)
  ! JPL: k_ClO_ClO   = k_3rd(temp,cair,1.6E-32,4.5,2.0E-12,2.4,0.6)
  k_BrO_NO2    = k_3rd_iupac(temp,cair,4.7E-31,3.1,1.8E-11,0.0,0.4)
  ! JPL: k_BrO_NO2   = k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)
  k_I_NO2      = k_3rd_iupac(temp,cair,3.0E-31,1.0,6.6E-11,0.0,0.63)
  ! for numerical reasons, the expression is multiplied by 1e30/1e30
  k_DMS_OH     = 1.E-9*EXP(5820./temp)*C(ind_O2)/ &
                 (1.E30+5.*EXP(6280./temp)*C(ind_O2))
  k_CH2OO_SO2  = 3.66E-11 ! average of 3.9E-11 + 3.42E-11
  k_O3s = (1.7E-12*EXP(-940./temp)) * C(ind_OH) &  ! <G2104>
        + (1.E-14*EXP(-490./temp)) * C(ind_HO2) &  ! <G2107>
        + jx(ip_O1D) * 2.2E-10 * C(ind_H2O) &      !
        / ( 3.2E-11*EXP(70./temp)*C(ind_O2)   &
           + 1.8E-11*EXP(110./temp)*C(ind_N2) &
           + 2.2E-10*C(ind_H2O) )
  ! new methane chemistry:
  ! branching ratio for methyl nitrate according to Butkovskaya et al.,
  ! (ref3177) but reduced according to Flocke et al. (ref3164)
  ! fit of data according to Lindemann-Hinshelwood scheme by J. Crowley
  ! http://iupac.pole-ether.fr/datasheets/pdf/R00_1_CH3O2_N0.pdf
  beta_null_CH3NO3 = 0.00295 + 5.15E-22*cair*(temp/298)**7.4
  beta_inf_CH3NO3  = 0.022
  beta_CH3NO3      = (beta_null_CH3NO3 * beta_inf_CH3NO3) /&
                     (beta_null_CH3NO3 + beta_inf_CH3NO3) / 10.
  k_NO2_CH3O2      = k_3rd(temp,cair,1.0E-30,4.8,7.2E-12,2.1,0.6)
  k_C6H5O2_NO2     = k_NO2_CH3O2 ! Consistent with ref3167 that set 1E-12 as lower limit at 298 K
and 1 bar.
  k_CH2OO_NO2          = 4.25E-12 ! average of 7.E-12 and 1.5E-12
  ! branching ratio for ethylnitrate formation according to Butkovskaya ref3170
  ! ratio transformed from beta = k1b/k1a to beta_C2H5NO3 = (1-(1+beta)^(-1))
  beta_C2H5NO3     = (1-1/(1+1.E-2*(3.88e-3*cair/2.46e19*760.+.365)*(1+1500.*(1/temp -1/298.))))
  ! ------------------------------------------------------------------------
  ! only for mim1, see mim1.rpl:
  ! op_kg_20110805+ for HO2 + NO -> HNO3 (butkovskaya_*.rpl)
  alpha_NO_HO2 = C(ind_H2O)*6.6E-27*temp*EXP(3700./temp)
  beta_NO_HO2  = MAX(((530./temp)+(press*4.8004E-6)-1.73)*0.01,0._dp)
  k0_NO_HO2    = 3.5E-12*EXP(250./temp)
  ! without humidity correction
  k2d_NO_HO2   = (beta_NO_HO2*k0_NO_HO2)/(1.+beta_NO_HO2)
  k1d_NO_HO2   = k0_NO_HO2 - k2d_NO_HO2
  ! with humidity correction
  k2w_NO_HO2   = (beta_NO_HO2*k0_NO_HO2*(1.+42.*alpha_NO_HO2))/ &
                 ((1.+alpha_NO_HO2)*(1.+beta_NO_HO2))
  k1w_NO_HO2   = k0_NO_HO2 - k2w_NO_HO2
  ! op_kg_20110805-
  k_Pr02_HO2   = 1.9E-13*EXP(1300./temp)
```

```
  k_Pr02_N0    = 2.7E-12*EXP(360./temp)
  k_Pr02_CH302 = 9.46E-14*EXP(431./temp)
  G7402a_yield = 0.8/1.1 ! 0.8+/-0.2
  ! end of mim1 block
  ! ------------------------------------------------------------------------
  k_CH3C03_N02 = k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6)
  k_PAN_M      = k_CH3C03_N02/(9.0E-29*EXP(14000./temp))
  ! rate coefficients from the MCM:
  KR02N0  = 2.54E-12*EXP(360./temp)
  KR02H02(:) = 2.91E-13*EXP(1300./temp)*(1.-EXP(-0.245*REAL(nC(:),dp))) ! ref1630
  KAPN0   = 8.10E-12*EXP(270./temp)  ! CH3C03 + N0
  KR02N03 = 2.50E-12
  KN03AL  = 1.4E-12*EXP(-1900./temp)
  ! updated rate constant for the RC03+H02 reactions
  ! (GroÃŸ, PhD Thesis, ref3195)
  ! except CH3C03+H02 that is taken from GroÃŸ ref3156
  KAPH02  = 5.20E-13*EXP(980./temp)*1.865 ! at 298K k(hoch2co3 + ho2) = 2.6(+-0.4)E-11 scaled with
IUPAC T-dependent expression
  ! Rate constants for the permutation reaction formalism
  ! calculated as in the permutation reaction formalism of MCM
  ! k_R02 = 2*(KR02self*k_CH302)^0.5
  ! k_R02self are taken from IUPAC recommendations unless noted otherwise
  k_CH302     = 1.03E-13*EXP(365./temp) ! CH302 + CH302 (IUPAC)
  ! Acyl peroxy radicals
  k_R02RC03   = 2.*2.E-12*EXP(500./temp) ! K17 for the CH302 + CH3C03 reaction directly taken from
ref. 1759. Old MCM value 1.00E-11 at 298 K.
  ! Alkyl radicals (unsubstituted, > C3)
  k_R02pR02   = 2.*(1.E-12*k_CH302)**(.5)                    ! Model compound (CH3)2CHCH202
(isobutyl, ref3210). Old MCM value 1.30E-12 at 298 K.
  k_R02sR02   = 2.*(1.6E-12*EXP(-2200./temp)*k_CH302)**(.5)! Model compound i-C3H702 (ref3175). Old
MCM value 2.50E-13 at 298 K.
  k_R02tR02   = 2.*3.8E-13*EXP(-1430./temp)              ! Model reaction t-C4H902 + CH302. Old
MCM value 6.70E-15 at 298 K.
  ! Alkyl radical with either O or Cl in beta
  k_R02pOR02  = 2.*7.5E-13*EXP(500./temp)                    ! Model reaction CH3COCH202 + CH302
(ref3175). Old MCM value 2.00E-12
  k_R02sOR02  = 2.*(7.7E-15*EXP(1330./temp)*k_CH302)**(.5) ! Model compound CH3CH(OH)CH(02)CH3
(ref3175). Old MCM value 8.80E-13 at 298 K.
  k_R02tOR02  = 2.*(4.7E-13*EXP(-1420./temp)*k_CH302)**(.5)    ! Model compound (CH3)2C(OH)C02(CH3)2
(ref3175). Old MCM value 9.20E-14 at 298 K.
  ! Allyl- and beta-hydroxy alkyl radicals
  k_R02LISOPAC02 = 2.*((2.8E-12+3.9E-12)/2.*k_CH302)**(.5)  ! Model compound ISOPA02 and ISOPC02.
Old MCM value 2.0E-12 at 298 K. K15 average from MCM ref. 2419
  k_R02ISOPB02   = 2.*(6.9E-14*k_CH302)**(.5)                ! Model compound ISOPB02. Old MCM
value 2.9E-12 at 298 K. K15 from MCM ref. 2419
  k_R02ISOPD02   = 2.*(4.8E-12*k_CH302)**(.5)                ! Model compound ISOPD02. Old MCM
value 8.0E-13 at 298 K. K15 from MCM ref. 2419
  ! T-dependent H-abstraction group rate constants
  k_p          = 4.49E-18*temp*temp*EXP(-320./temp) ! Kwok and Atkinson, ref3194
  k_s          = 4.50E-18*temp*temp*EXP(253./temp)  ! Kwok and Atkinson, ref3194
  k_t          = 2.12E-18*temp*temp*EXP(696./temp)  ! Kwok and Atkinson, ref3194
  k_rohro      = 2.1E-18*temp*temp*EXP(-85./temp)   ! Kwok and Atkinson, ref3194
  k_co2h       = .7*4.2E-14*EXP(850./temp)          ! CH3C02H + OH = CH3C02, ref1759
  ! T-dependent OH-addition rate constants
  k_adp        = 4.5E-12*(temp/300.)**(-0.85)                        ! 1/2 k(OH + C2H4), high
pressure limit IUPAC as in Peeters et al. 2007
  k_ads        = .25*(1.1E-11*EXP(485./temp)+1.0E-11*EXP(553./temp)) ! 1/2 * k_av(OH + cis/trans 2-
butene) as in Peeters et al. 2007
  k_adt        = 1.922E-11*EXP(450./temp) - k_ads                    ! k(OH + 2-methyl-2-butene) -
k_ads
  KHSB         = 1.52E11*EXP(-9512./temp)*1. ! 1,5-H-shift Peeters et al(2009) 0.003533 s-1 at 303K
  KHSD         = 6.08E10*EXP(-8893./temp)*1. ! 1,5-H-shift Peeters et al(2009) 0.0109 s-1 at 303K
  ! 1,6-H-shift for ZIS0PA02 and ZIS0PC02
  K16HSZ14     = 2.28E9 * exp(-6764/temp) * 0.28 ! 0.07035 s-1 at 295K ! as in SI Taraborrelli et
al., Nat. Geosc. 2012
  K16HSZ41     = 1.23E9 * exp(-6186/temp) * 0.28 ! 0.2692 s-1 at 295K
  K16HS        = (K16HSZ14*K16HSZ41)**(.5)
  K15HSDHB     = 5.                                  ! 1,5-H-shift assisted by double H-bonding after
Peeters and MÃ¼ller(2010)
  ! 1,4-H-shift involving an aldehydic hydrogen
  !  K14HSAL = 2.9E7*exp(-5297/temp) ! Crounse et al. JPC A (2012) barrier 19.0 kcal/mol => ~ 0.5 s-
1 at 295K
  K14HSAL      = 2.9E7*exp(-1*(5297+705)/temp) ! CCSD(T)/aug-Schartz4(DT)//M05-2X/6-311G(d,p))
yields a barrier of 20.39 (L. Vereecken 2013) => ~ 0.04 s-1 at 295K
  K15HS24VYNAL = K16HSZ14 * exp(-3500/(1.987*temp)) ! adding 3.5 kcal to the barrier of 1,6-H-shift
as from SAR by L. Vereecken
  K15HS42VYNAL = K16HSZ41 * exp(-3500/(1.987*temp))
  KHYDEC       = 6.e14*exp(-16000./(1.98588*temp)) ! in cal Ea from Nguyen et al(2009) A from Baulch
et al(2005)
  ! Rate constants for the formic acid production via vinyl alcohol. Also used for some bigger and
saturated aldehydes.
  k_CH2CH0H_0H_HC00H = 4.3E-11 ! ref3179
  k_CH2CH0H_0H_ALD   = 2.4E-11 ! ref3179
  k_CH2CH0H_HC00H    = 4.67E-26*temp**3.286*EXP(4509./(1.987*temp)) ! ref3162
  k_ALD_HC00H        = 1.17E-19*temp**1.209*EXP(-556./(1.987*temp)) ! ref3162
  J_IC3H7N03   = 3.7*jx(ip_PAN)
  J_ACET0L     = 0.65*0.11*jx(ip_CH0H)
  J_HPALD      = (JX(IP_CH300H)+ JX(ip_MACR)/0.004)
  J_KETENE     = jx(ip_MVK)/0.004
  R02 = 0.
  IF (ind_LIS0PAC02>0)           R02 = R02 + C(ind_LIS0PAC02)
  IF (ind_LDIS0PAC02>0)          R02 = R02 + C(ind_LDIS0PAC02)
  IF (ind_IS0PB02>0)             R02 = R02 + C(ind_IS0PB02)
  IF (ind_IS0PD02>0)             R02 = R02 + C(ind_IS0PD02)
  IF (ind_LIS0PEF02>0)           R02 = R02 + C(ind_LIS0PEF02)
  IF (ind_NIS0P02>0)             R02 = R02 + C(ind_NIS0P02)
  IF (ind_LHC4ACC03>0)           R02 = R02 + C(ind_LHC4ACC03)
  IF (ind_LC57802>0)             R02 = R02 + C(ind_LC57802)
  IF (ind_C5902>0)               R02 = R02 + C(ind_C5902)
  IF (ind_LNIS03>0)              R02 = R02 + C(ind_LNIS03)
  IF (ind_CH302>0)               R02 = R02 + C(ind_CH302)
  IF (ind_H0CH202>0)             R02 = R02 + C(ind_H0CH202)
  IF (ind_CH3C03>0)              R02 = R02 + C(ind_CH3C03)
  IF (ind_C2H502>0)              R02 = R02 + C(ind_C2H502)
  IF (ind_H0CH2C03>0)            R02 = R02 + C(ind_H0CH2C03)
  IF (ind_HYPR0P02>0)            R02 = R02 + C(ind_HYPR0P02)
  IF (ind_LBUT1EN02>0)           R02 = R02 + C(ind_LBUT1EN02)
  IF (ind_BUT20L02>0)            R02 = R02 + C(ind_BUT20L02)
  IF (ind_HC0C03>0)              R02 = R02 + C(ind_HC0C03)
  IF (ind_C02H3C03>0)            R02 = R02 + C(ind_C02H3C03)
  IF (ind_LHMVKAB02>0)           R02 = R02 + C(ind_LHMVKAB02)
  IF (ind_MAC03>0)               R02 = R02 + C(ind_MAC03)
  IF (ind_MACR02>0)              R02 = R02 + C(ind_MACR02)
  IF (ind_PR0N03B02>0)           R02 = R02 + C(ind_PR0N03B02)
  IF (ind_H0CH2CH202>0)          R02 = R02 + C(ind_H0CH2CH202)
  IF (ind_CH3C0CH202>0)          R02 = R02 + C(ind_CH3C0CH202)
  IF (ind_IC3H702>0)             R02 = R02 + C(ind_IC3H702)
  IF (ind_NC3H702>0)             R02 = R02 + C(ind_NC3H702)
  IF (ind_LC4H902>0)             R02 = R02 + C(ind_LC4H902)
  IF (ind_TC4H902>0)             R02 = R02 + C(ind_TC4H902)
  IF (ind_LMEK02>0)              R02 = R02 + C(ind_LMEK02)
  IF (ind_HC0CH202>0)            R02 = R02 + C(ind_HC0CH202)
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IF (ind_EZCH3C02CHCH0>0)        R02 = R02 + C(ind_EZCH3C02CHCH0)
IF (ind_EZCH0CCH3CH02>0)        R02 = R02 + C(ind_EZCH0CCH3CH02)
IF (ind_CH3C0CH02CH0>0)         R02 = R02 + C(ind_CH3C0CH02CH0)
IF (ind_HC0C02CH3CH0>0)         R02 = R02 + C(ind_HC0C02CH3CH0)
IF (ind_C10DC302C400H>0)        R02 = R02 + C(ind_C10DC302C400H)
IF (ind_C100HC202C40D>0)        R02 = R02 + C(ind_C100HC202C40D)
IF (ind_C10DC202C40D>0)         R02 = R02 + C(ind_C10DC202C40D)
IF (ind_IS0PBDN0302>0)          R02 = R02 + C(ind_IS0PBDN0302)
IF (ind_LIS0PACN0302>0)         R02 = R02 + C(ind_LIS0PACN0302)
IF (ind_DB102>0)                R02 = R02 + C(ind_DB102)
IF (ind_DB202>0)                R02 = R02 + C(ind_DB202)
IF (ind_LME3FURAN02>0)          R02 = R02 + C(ind_LME3FURAN02)
IF (ind_N03CH2C03>0)            R02 = R02 + C(ind_N03CH2C03)
IF (ind_CH3C0C03>0)             R02 = R02 + C(ind_CH3C0C03)
IF (ind_ZC03C23DBC0D>0)         R02 = R02 + C(ind_ZC03C23DBC0D)
IF (ind_IBUT0LB02>0)            R02 = R02 + C(ind_IBUT0LB02)
IF (ind_IPRC03>0)               R02 = R02 + C(ind_IPRC03)
IF (ind_IC4H902>0)              R02 = R02 + C(ind_IC4H902)
! MB0-related
IF (ind_LMB0AB02>0)             R02 = R02 + C(ind_LMB0AB02)
IF (ind_IPRH0C03>0)             R02 = R02 + C(ind_IPRH0C03)
IF (ind_LNMB0AB02>0)            R02 = R02 + C(ind_LNMB0AB02)
IF (ind_NC40HC03>0)             R02 = R02 + C(ind_NC40HC03)
! APINENE-related:
IF (ind_LAPINAB02>0)            R02 = R02 + C(ind_LAPINAB02)
IF (ind_C96O2>0)                R02 = R02 + C(ind_C96O2)
IF (ind_C97O2>0)                R02 = R02 + C(ind_C97O2)
IF (ind_C98O2>0)                R02 = R02 + C(ind_C98O2)
IF (ind_C85O2>0)                R02 = R02 + C(ind_C85O2)
IF (ind_C86O2>0)                R02 = R02 + C(ind_C86O2)
IF (ind_PINAL02>0)              R02 = R02 + C(ind_PINAL02)
IF (ind_C96C03>0)               R02 = R02 + C(ind_C96C03)
IF (ind_C89C03>0)               R02 = R02 + C(ind_C89C03)
IF (ind_C85C03>0)               R02 = R02 + C(ind_C85C03)
IF (ind_0HMENTHEN6ONE02>0)      R02 = R02 + C(ind_0HMENTHEN6ONE02)
IF (ind_C5110O2>0)              R02 = R02 + C(ind_C5110O2)
IF (ind_C10O6O2>0)              R02 = R02 + C(ind_C10O6O2)
IF (ind_C0235C6C03>0)           R02 = R02 + C(ind_C0235C6C03)
IF (ind_CH0C3C0C03>0)           R02 = R02 + C(ind_CH0C3C0C03)
IF (ind_C0235C6O2>0)            R02 = R02 + C(ind_C0235C6O2)
IF (ind_C716O2>0)               R02 = R02 + C(ind_C716O2)
IF (ind_C61402>0)               R02 = R02 + C(ind_C61402)
IF (ind_HC0CH2C03>0)            R02 = R02 + C(ind_HC0CH2C03)
IF (ind_BIACET02>0)             R02 = R02 + C(ind_BIACET02)
IF (ind_C023C4C03>0)            R02 = R02 + C(ind_C023C4C03)
IF (ind_C10902>0)               R02 = R02 + C(ind_C10902)
IF (ind_C811C03>0)              R02 = R02 + C(ind_C811C03)
IF (ind_C8902>0)                R02 = R02 + C(ind_C8902)
IF (ind_C81202>0)               R02 = R02 + C(ind_C81202)
IF (ind_C81302>0)               R02 = R02 + C(ind_C81302)
IF (ind_C721C03>0)              R02 = R02 + C(ind_C721C03)
IF (ind_C72102>0)               R02 = R02 + C(ind_C72102)
IF (ind_C72202>0)               R02 = R02 + C(ind_C72202)
IF (ind_C4402>0)                R02 = R02 + C(ind_C4402)
IF (ind_C51202>0)               R02 = R02 + C(ind_C51202)
IF (ind_C51302>0)               R02 = R02 + C(ind_C51302)
IF (ind_CH0C3C002>0)            R02 = R02 + C(ind_CH0C3C002)
IF (ind_C312C0C03>0)            R02 = R02 + C(ind_C312C0C03)
IF (ind_H0C2H4C03>0)            R02 = R02 + C(ind_H0C2H4C03)
IF (ind_LNAPINAB02>0)           R02 = R02 + C(ind_LNAPINAB02)
IF (ind_C81002>0)               R02 = R02 + C(ind_C81002)
IF (ind_C51402>0)               R02 = R02 + C(ind_C51402)
IF (ind_CH0C0CH202>0)           R02 = R02 + C(ind_CH0C0CH202)
! BPINENE-related:
IF (ind_R006R102>0)             R02 = R02 + C(ind_R006R102)
IF (ind_R006R302>0)             R02 = R02 + C(ind_R006R302)
IF (ind_R06R102>0)              R02 = R02 + C(ind_R06R102)
IF (ind_R06R302>0)              R02 = R02 + C(ind_R06R302)
IF (ind_BPINA02>0)              R02 = R02 + C(ind_BPINA02)
IF (ind_C8BC02>0)               R02 = R02 + C(ind_C8BC02)
IF (ind_N0PIND02>0)             R02 = R02 + C(ind_N0PIND02)
IF (ind_LNBPINAB02>0)           R02 = R02 + C(ind_LNBPINAB02)
! aromatics-related:
IF (ind_BZBIPER02>0)            R02 = R02 + C(ind_BZBIPER02)
IF (ind_C6H5CH202>0)            R02 = R02 + C(ind_C6H5CH202)
IF (ind_TLBIPER02>0)            R02 = R02 + C(ind_TLBIPER02)
IF (ind_BZEMUCC03>0)            R02 = R02 + C(ind_BZEMUCC03)
IF (ind_BZEMUC02>0)             R02 = R02 + C(ind_BZEMUC02)
IF (ind_C5DIAL02>0)             R02 = R02 + C(ind_C5DIAL02)
IF (ind_NPHEN02>0)              R02 = R02 + C(ind_NPHEN02)
IF (ind_PHEN02>0)               R02 = R02 + C(ind_PHEN02)
IF (ind_CRES02>0)               R02 = R02 + C(ind_CRES02)
IF (ind_NCRES02>0)              R02 = R02 + C(ind_NCRES02)
IF (ind_TLEMUCC03>0)            R02 = R02 + C(ind_TLEMUCC03)
IF (ind_TLEMUC02>0)             R02 = R02 + C(ind_TLEMUC02)
IF (ind_C615C0202>0)            R02 = R02 + C(ind_C615C0202)
IF (ind_MALDIALC03>0)           R02 = R02 + C(ind_MALDIALC03)
IF (ind_EPXDLC03>0)             R02 = R02 + C(ind_EPXDLC03)
IF (ind_C3DIAL02>0)             R02 = R02 + C(ind_C3DIAL02)
IF (ind_MALDIAL02>0)            R02 = R02 + C(ind_MALDIAL02)
IF (ind_C6H502>0)               R02 = R02 + C(ind_C6H502)
IF (ind_C6H5C03>0)              R02 = R02 + C(ind_C6H5C03)
IF (ind_0XYL102>0)              R02 = R02 + C(ind_0XYL102)
IF (ind_C5C01402>0)             R02 = R02 + C(ind_C5C01402)
IF (ind_NBZFU02>0)              R02 = R02 + C(ind_NBZFU02)
IF (ind_BZFU02>0)               R02 = R02 + C(ind_BZFU02)
IF (ind_HC0C0HC03>0)            R02 = R02 + C(ind_HC0C0HC03)
IF (ind_CATEC102>0)             R02 = R02 + C(ind_CATEC102)
IF (ind_MCATEC102>0)            R02 = R02 + C(ind_MCATEC102)
IF (ind_C5DICARB02>0)           R02 = R02 + C(ind_C5DICARB02)
IF (ind_NTLFU02>0)              R02 = R02 + C(ind_NTLFU02)
IF (ind_TLFU02>0)               R02 = R02 + C(ind_TLFU02)
IF (ind_NPHEN102>0)             R02 = R02 + C(ind_NPHEN102)
IF (ind_NNCATEC02>0)            R02 = R02 + C(ind_NNCATEC02)
IF (ind_NCATEC02>0)             R02 = R02 + C(ind_NCATEC02)
IF (ind_NBZ002>0)               R02 = R02 + C(ind_NBZ002)
IF (ind_PBZ002>0)               R02 = R02 + C(ind_PBZ002)
IF (ind_NPTL002>0)              R02 = R02 + C(ind_NPTL002)
IF (ind_PTL002>0)               R02 = R02 + C(ind_PTL002)
IF (ind_NCRES102>0)             R02 = R02 + C(ind_NCRES102)
IF (ind_MNNCATEC02>0)           R02 = R02 + C(ind_MNNCATEC02)
IF (ind_MNCATEC02>0)            R02 = R02 + C(ind_MNCATEC02)
IF (ind_MEC0ACET02>0)           R02 = R02 + C(ind_MEC0ACET02)
IF (ind_C02H3C03>0)             R02 = R02 + C(ind_C02H3C03)
IF (ind_MALANHY02>0)            R02 = R02 + C(ind_MALANHY02)
IF (ind_NDNPHEN02>0)            R02 = R02 + C(ind_NDNPHEN02)
IF (ind_DNPHEN02>0)             R02 = R02 + C(ind_DNPHEN02)
IF (ind_NDNCRES02>0)            R02 = R02 + C(ind_NDNCRES02)
IF (ind_DNCRES02>0)             R02 = R02 + C(ind_DNCRES02)
IF (ind_C5C020HC03>0)           R02 = R02 + C(ind_C5C020HC03)
IF (ind_C6C020HC03>0)           R02 = R02 + C(ind_C6C020HC03)
IF (ind_MMALANHY02>0)           R02 = R02 + C(ind_MMALANHY02)
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  IF (ind_ACCOMEC03>0)            RO2 = RO2 + C(ind_ACCOMEC03)
  IF (ind_C4CO2DBC03>0)           RO2 = RO2 + C(ind_C4CO2DBC03)
  IF (ind_C5CO2DBC03>0)           RO2 = RO2 + C(ind_C5CO2DBC03)
  IF (ind_NSTYREN02>0)            RO2 = RO2 + C(ind_NSTYREN02)
  IF (ind_STYREN02>0)             RO2 = RO2 + C(ind_STYREN02)
  ! pseudo first order rate constants    ! occurence
  k1_RO2RC03      = RO2 * k_RO2RC03      ! 51
  k1_RO2pR02      = RO2 * k_RO2pR02      ! 5
  k1_RO2sR02      = RO2 * k_RO2sR02      ! 11+1
  k1_RO2tR02      = RO2 * k_RO2tR02      ! 13+1
  k1_RO2p0R02     = RO2 * k_RO2p0R02     ! 11+2
  k1_RO2s0R02     = RO2 * k_RO2s0R02     ! 33+2
  k1_RO2t0R02     = RO2 * k_RO2t0R02     ! 17
  k1_RO2LIS0PAC02 = RO2 * k_RO2LIS0PAC02 ! 3
  k1_RO2IS0PB02   = RO2 * k_RO2IS0PB02   ! 1
  k1_RO2IS0PD02   = RO2 * k_RO2IS0PD02   ! 13
#ENDINLINE {above lines go into the SUBROUTINES UPDATE_RCONST and UPDATE_PHOTO}
#INLINE F90_RATES
  ELEMENTAL REAL(dp) FUNCTION k_SIV_H202 (k_298,tdep,cHp,temp)
    ! special rate function for S(IV) + H2O2
    REAL,     INTENT(IN) :: k_298 ! k at T = 298.15K
    REAL,     INTENT(IN) :: tdep  ! temperature dependence
    REAL(dp), INTENT(IN) :: cHp   ! c(H+)
    REAL(dp), INTENT(IN) :: temp  ! temperature
    INTRINSIC :: EXP
    k_SIV_H202 = k_298 * EXP(tdep*(1._dp/temp-3.3540E-3_dp)) &
      * cHp / (cHp+0.1_dp)
  END FUNCTION k_SIV_H202
  ELEMENTAL REAL(dp) FUNCTION k_3rd_iupac(temp,cair,k0_300K,n,kinf_300K,m,fc)
    ! IUPAC three body reaction formula (iupac.pole-ether.fr)
    INTRINSIC :: LOG10
    REAL(dp), INTENT(IN) :: temp      ! temperature [K]
    REAL(dp), INTENT(IN) :: cair      ! air concentration [molecules/cm3]
    REAL,     INTENT(IN) :: k0_300K   ! low pressure limit at 300 K
    REAL,     INTENT(IN) :: n         ! exponent for low pressure limit
    REAL,     INTENT(IN) :: kinf_300K ! high pressure limit at 300 K
    REAL,     INTENT(IN) :: m         ! exponent for high pressure limit
    REAL,     INTENT(IN) :: fc        ! broadening factor (e.g. 0.45 or 0.6...)
    REAL                 :: nu        ! N
    REAL                 :: zt_help, k0_T, kinf_T, k_ratio
    zt_help = 300._dp/temp
    k0_T    = k0_300K   * zt_help**(n) * cair ! k_0   at current T
    kinf_T  = kinf_300K * zt_help**(m)        ! k_inf at current T
    k_ratio = k0_T/kinf_T
    nu      = 0.75-1.27*LOG10(fc)
    k_3rd_iupac = k0_T/(1._dp+k_ratio)* &
      fc**(1._dp/(1._dp+(LOG10(k_ratio)/nu)**2))
  END FUNCTION k_3rd_iupac
  ELEMENTAL REAL(dp) FUNCTION alpha_AN(n,ro2type,bcarb,gcarb,abic,temp,cair)
  ! Alkyl nitrate yields dependent on T and P according to
  ! Arey. ref3202 and Teng, ref3189
    INTRINSIC :: LOG10
    INTEGER,  INTENT(IN) :: n         ! number of heavy atoms (C, O, N) except the O atom of beta-
carbonyls
    INTEGER,  INTENT(IN) :: ro2type   ! 1, 2 or 3 for primary, secondary and tertiary RO2
    INTEGER,  INTENT(IN) :: bcarb     ! 1 for beta-carbonyl group, 0 for none
    INTEGER,  INTENT(IN) :: gcarb     ! 1 for gamma-carbonyl group, 0 for none
    INTEGER,  INTENT(IN) :: abic      ! 1 for bicyclic peroxy from aromatics, 0 for none
    REAL(dp), INTENT(IN) :: temp      ! temperature [K]
    REAL(dp), INTENT(IN) :: cair      ! air concentration [molecules/cm3]
    REAL(dp), PARAMETER  :: alpha=2.E-22, beta=1.0, Yinf_298K=0.43, F=0.41, m0=0., minf=8.0
    REAL(dp)             :: m           ! factor for primary, secondary and tertiary RO2
    REAL(dp)             :: bcf,gcf,abf ! reduction factors for the presence of beta-carbonyl and
gamma-carbonyl group and a bicyclic peroxy from aromatics
    REAL(dp)             :: rtemp,rcair,Y0_298K, Y0_298K_tp, Yinf_298K_t, zeta, k_ratio
    m = 1. ! According to Teng, ref3189
    IF (bcarb .EQ. 1) THEN
      bcf = 0.19 ! derived from Praske, ref3190: alpha_AN = 0.03 for the secondary HMK02 relative to
alpha_AN for 6C RO2 (0.16)
    ELSE IF (bcarb .EQ. 0) THEN
      bcf = 1.
    ELSE
      bcf = 1.
    ENDIF
    IF (gcarb .EQ. 1) THEN
      gcf = 0.44 ! derived from Praske, ref3190: alpha_AN = 0.07 for the primary HMK02 relative to
alpha_AN for 6C RO2 (0.16)
    ELSE IF (gcarb .EQ. 0) THEN
      gcf = 1.
    ELSE
      gcf = 1.
    ENDIF
    IF (abic .EQ. 1) THEN
      abf = 0.24 ! derived from the ratio of AN-yield for toluene from Elrod et al. (ref3180), 5.5%
at 200 torr, and this SAR for linear alkyl RO2 with 9 heavy atoms, 23.3%
    ELSE IF (abic .EQ. 0) THEN
      abf = 1.
    ENDIF
    rtemp = temp
    rcair = cair
    ! or like in other atmospheric models
    ! rtemp = 298.
    ! rcair = 2.46E19
    Y0_298K     = alpha*EXP(beta*n)
    Y0_298K_tp  = Y0_298K * cair * (rtemp/298)**(-m0)
    Yinf_298K_t = Yinf_298K * (rtemp/298)**(-minf)
    zeta        = 1/(1+LOG10(Y0_298K_tp/Yinf_298K_t)**2)
    k_ratio     = (Y0_298K_tp/(1+Y0_298K_tp/Yinf_298K_t))*F**zeta
    alpha_AN    = k_ratio/(1+k_ratio) * m * bcf * gcf * abf
  END FUNCTION alpha_AN
  ELEMENTAL REAL(dp) FUNCTION k_limited (k3rd,cHp)
    ! diffusion limitation caps 3rd order rate coefficients
    REAL(dp), INTENT(IN) :: k3rd  ! 3rd order rate coefficient
    REAL(dp), INTENT(IN) :: cHp   ! c(H+)
    REAL(dp), PARAMETER  :: DiffLimit = 1E10 ! diffusion limitation [M-1s-1]
    INTRINSIC :: EXP
    k_limited = 1._dp / ( 1._dp/k3rd + cHp/DiffLimit)
  END FUNCTION k_limited
  ELEMENTAL REAL(dp) FUNCTION k_N2_0(temp,temp_ion)
    REAL(dp), INTENT(IN) :: temp      ! temperature [K]
    REAL(dp), INTENT(IN) :: temp_ion  ! ion temperature [K]
    REAL                 :: temp_mean
    temp_mean = (temp_ion + temp)/2
    k_N2_0 = 1.4E-10*(300./temp_mean)**0.44
  END FUNCTION k_N2_0
  ELEMENTAL REAL(dp) FUNCTION k_0p_02(temp,temp_ion)
    REAL(dp), INTENT(IN) :: temp      ! temperature [K]
    REAL(dp), INTENT(IN) :: temp_ion  ! ion temperature [K]
    REAL(dp)             :: temp_mean
    temp_mean  = .667*temp_ion + .333*temp
    k_0p_02  = 2.82E-11 - 7.74E-12*(temp_mean/300.) + &
      1.073E-12*(temp_mean/300.)**2 - 5.17E-14*(temp_mean/300.)**3 + &
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      9.65E-16*(temp_mean/300.)**4
  END FUNCTION k_0p_02
  ELEMENTAL REAL(dp) FUNCTION k_0p_N2(temp,temp_ion)
    REAL(dp), INTENT(IN) :: temp      ! temperature [K]
    REAL(dp), INTENT(IN) :: temp_ion  ! ion temperature [K]
    REAL(dp)             :: temp_mean
    temp_mean = .6363*temp_ion + .3637*temp
    k_0p_N2 = 1.533E-12 - 5.92E-13*(temp_mean/300.) + 8.6E-14*(temp_mean/300.)**2
  END FUNCTION k_0p_N2
#ENDINLINE {above lines go into MODULE messy_mecca_kpp_Rates}

#INLINE F90_GLOBAL
  ! from xmecca:
  LOGICAL, PARAMETER :: REQ_HET     = .TRUE.
  LOGICAL, PARAMETER :: REQ_PHOTRAT = .TRUE.
  LOGICAL, PARAMETER :: REQ_AEROSOL = .FALSE.
#ENDINLINE {above lines go to messy_mecca_kpp_global}
#INLINE F90_GLOBAL
  ! from xmecca:
  INTEGER, PARAMETER, PUBLIC :: MAX_MCEXP = 1
!KPPPP_DIRECTIVE vector variable definition start
  REAL :: mcexp(MAX_MCEXP) ! dummy Monte-Carlo factor
!KPPPP_DIRECTIVE vector variable definition end
#ENDINLINE {above lines go to messy_mecca_kpp_global}

#EQUATIONS
{<G1nnn> ------------------------------ O -------------------------}{@\myhline}
<G1000>  O2   + O1D      = O3P + O2   {+ 189. kJmol} : {%UpStTrG} 3.3E-11*EXP(55./temp); {&2626}
<G1001>  O2   + O3P {+M} = O3                        : {%UpStTrG} 6.E-34*((temp/300.)**(-2.4))*cair; {&2626}
<G1002a> O3   + O1D      = 2 O2                      : {%UpStG}   1.2E-10; {&2626} // The path leading to 2 \kpp{O3P} + \kpp{O2} results in a null cycle regarding odd oxygen and is neglected.
<G1002> O3   + O3P      = 2 O2       {+ 392. kJmol} : {%UpStG}   8.E-12*EXP(-2060./temp); {&2626}
{<G2nnn> ------------------------------ H -------------------------}{@\myhline}
<G2100>  H    + O2 {+M}  = HO2        {+ 204. kJmol} : {%UpStTrG} k_3rd(temp,cair,4.4E-32,1.3,7.5E-11,-0.2,0.6); {&2626}
<G2101>  H    + O3       = OH + O2    {+ 119. kJmol} : {%UpStG}   1.4E-10*EXP(-470./temp); {&2626}
<G2102>  H2   + O1D      = H + OH     {+ 181. kJmol} : {%UpStG}   1.2E-10; {&2626}
<G2103>  OH   + O3P      = H + O2     {+ 69.5 kJmol} : {%UpStG}   1.8E-11*EXP(180./temp); {&2626}
<G2104>  OH   + O3       = HO2 + O2   {+ 167. kJmol} : {%UpStTrG} 1.7E-12*EXP(-940./temp); {&2626}
<G2105>  OH   + H2       = H2O + H    {+ 62.7 kJmol} : {%UpStTrG} 2.8E-12*EXP(-1800./temp); {&2626}
<G2106>  HO2  + O3P      = OH + O2    {+ 225. kJmol} : {%UpStG}   3.E-11*EXP(200./temp); {&2626}
<G2107>  HO2  + O3       = OH + 2 O2  {+ 119. kJmol} : {%UpStTrG} 1.E-14*EXP(-490./temp); {&2626}
<G2108a> HO2  + H        = 2 OH       {+ 155. kJmol} : {%UpStG}   7.2E-11; {&2626}
<G2108b> HO2  + H        = H2 + O2    {+ 233. kJmol} : {%UpStG}   6.9E-12; {&2626}
<G2108c> HO2  + H        = O3P + H2O  {+ 226. kJmol} : {%UpStG}   1.6E-12; {&2626}
<G2109>  HO2  + OH       = H2O + O2   {+ 295. kJmol} : {%UpStTrG} 4.8E-11*EXP(250./temp); {&2626}
<G2110>  HO2  + HO2      = H2O2 + O2  {+ 165. kJmol} : {%UpStTrG} k_HO2_HO2; {&1599, 165} // The rate coefficient is: \code{k_HO2_HO2} = \code{(1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))}. The value for the first (pressure-independent) part is from \citet{1599}, the water term from \citet{165}.
<G2111>  H2O  + O1D      = 2 OH       {+ 119. kJmol} : {%UpStTrG} 1.63E-10*EXP(60./temp); {&2626}
<G2112>  H2O2 + OH       = H2O + HO2  {+ 130. kJmol} : {%UpStTrG} 1.8E-12; {&2626}
<G2117>  H2O  + H2O      = H2OH2O                    : {%UpStTrG} 6.521E-26*temp*EXP(1851.09/temp)*EXP(-5.10485E-3*temp); {&3052} // Converted to Kc [molec-1 cm3]= Kp*R*T/NA, where R is 82.05736 [cm3â€‰atmâ€‰Kâ¯¹â€‰molâ¯¹].
<G2118>  H2OH2O          = H2O  + H2O                : {%UpStTrG} 1.E0; // Assuming fast equilibrium.
{<G3nnn> ------------------------------ N -------------------------}{@\myhline}
<G3100>  N    + O2       = NO + O3P   {+ 135. kJmol}  : {%UpStG}   1.5E-11*EXP(-3600./temp); {&2626}
<G3101>  N2   + O1D      = O3P + N2   {+ 189. kJmol}  : {%UpStTrG} 2.15E-11*EXP(110./temp); {&2626}
<G3102a> N2O  + O1D      = 2 NO       {+ 197. kJmol}  : {%UpStG}   7.25E-11*EXP(20./temp); {&2626}
<G3102b> N2O  + O1D      = N2 + O2                    : {%StG}    4.63E-11*EXP(20./temp); {&2626}
<G3103>  NO   + O3       = NO2 + O2   {+ 201. kJmol}  : {%UpStTrG} 3.E-12*EXP(-1500./temp); {&2626}
<G3104>  NO   + N        = O3P + N2   {+ 259. kJmol}  : {%UpStG}   2.1E-11*EXP(100./temp); {&2626}
<G3105>  NO2  + O3P      = NO + O2    {+ 191. kJmol}  : {%UpStG}   5.1E-12*EXP(210./temp); {&2626}
<G3106>  NO2  + O3       = NO3 + O2                   : {%StTrG}  1.2E-13*EXP(-2450./temp); {&2626}
<G3107>  NO2  + N        = N2O + O3P  {+ 104. kJmol}  : {%UpStG}   5.8E-12*EXP(220./temp); {&2626}
<G3108>  NO3  + NO       = 2 NO2                      : {%StTrG}  1.5E-11*EXP(170./temp); {&2626}
<G3109>  NO3  + NO2 {+M} = N2O5                       : {%UpStTrG} k_NO3_NO2; {&2626} // The rate coefficient is: \code{k_NO3_NO2} = \code{k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6)}.
<G3110>  N2O5       {+M} = NO2 + NO3                 : {%StTrG}  k_NO3_NO2/(2.7E-27*EXP(11000./temp)); {&2626} // The rate coefficient is defined as backward reaction divided by equilibrium constant.
<G3200>  NO   + OH {+M}  = HONO          : {%TrG}   k_3rd(temp,cair,7.0E-31,2.6,3.6E-11,0.1,0.6); {&2626}
<G3201>  NO   + HO2      = NO2   + OH {+ 33.8 kJmol} : {%UpStTrG} 3.3E-12*EXP(270./temp); {&2626}
<G3202>  NO2  + OH  {+M} = HNO3          : {%UpStTrG} k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0.,0.6); {&2626}
<G3203>  NO2  + HO2 {+M} = HNO4          : {%StTrG} k_NO2_HO2; {&2626} // The rate coefficient is: \code{k_NO2_HO2} = \code{k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)}.
<G3204>  NO3  + HO2      = NO2 + OH + O2 : {%TrG}   3.5E-12; {&2626}
<G3205>  HONO + OH       = NO2 + H2O     : {%TrG}   1.8E-11*EXP(-390./temp); {&2626}
<G3206>  HNO3 + OH       = H2O   + NO3   : {%StTrG} k_HNO3_OH; {&2626} // The rate coefficient is: \code{k_HNO3_OH} = \code{2.4E-14 * EXP(460./temp) + 1./ ( 1./(6.5E-34 * EXP(1335./temp)*cair) + 1./(2.7E-17 * EXP(2199./temp)) )}
<G3207>  HNO4       {+M} = NO2   + HO2   : {%StTrG} k_NO2_HO2/(2.1E-27*EXP(10900./temp)); {&2626} // The rate coefficient is defined as backward reaction divided by equilibrium constant.
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<G3208>  HNO4 + OH       = NO2   + H2O   : {%StTrG} 1.3E-12*EXP(380./temp); {&2626}
<G3209>  NH3   + OH      = NH2 + H2O     : {%TrG}   1.7E-12*EXP(-710./temp); {&2415}
<G3210>  NH2   + O3      = NH2O + O2     : {%TrG}   4.3E-12*EXP(-930./temp); {&2415}
<G3211>  NH2   + HO2     = NH2O + OH     : {%TrG}   4.8E-07*EXP(-628./temp)*temp**(-1.32); {&2415}
<G3212>  NH2   + HO2     = HNO + H2O     : {%TrG}   9.4E-09*EXP(-356./temp)*temp**(-1.12); {&2415}
<G3213>  NH2   + NO      = HO2 + OH + N2 : {%TrG}   1.92E-12*((temp/298.)**(-1.5)); {&2415}
<G3214>  NH2   + NO      = N2 + H2O      : {%TrG}   1.41E-11*((temp/298.)**(-1.5)); {&2415}
<G3215>  NH2   + NO2     = N2O + H2O     : {%TrG}   1.2E-11*((temp/298.)**(-2.0)); {&2415}
<G3216>  NH2   + NO2     = NH2O + NO     : {%TrG}   0.8E-11*((temp/298.)**(-2.0)); {&2415}
<G3217>  NH2O  + O3      = NH2 + O2      : {%TrG}   1.2E-14; {&2415}
<G3218>  NH2O            = NHOH          : {%TrG}   1.3E3; {&2415}
<G3219>  HNO   + OH      = NO + H2O      : {%TrG}   8.0E-11*EXP(-500./temp); {&2415}
<G3220>  HNO   + NHOH    = NH2OH + NO    : {%TrG}   1.66E-12*EXP(-1500./temp); {&2415}
<G3221>  HNO   + NO2     = HONO + NO     : {%TrG}   1.0E-12*EXP(-1000./temp); {&2415}
<G3222>  NHOH  + OH      = HNO + H2O     : {%TrG}   1.66E-12; {&2415}
<G3223>  NH2OH + OH      = NHOH + H2O    : {%TrG}   4.13E-11*EXP(-2138./temp); {&2415}
<G3224>  HNO   + O2      = HO2 + NO      : {%TrG}   3.65E-14*EXP(-4600./temp); {&2415}
{<G4nnn> ---------------------------- C ------------------------}{@\myhline}
<G4100>  CH4       + O1D      = .75 CH3 + .75 OH + .25 HCHO + .4 H + .05 H2 {+ 438. kJmol} : {%UpStG} 1.75E-10; {&2626}
<G4101>  CH4       + OH       = CH3 + H2O          : {%StTrG} 1.85E-20*EXP(2.82*LOG(temp)-987./temp); {&1627}
<G4102>  CH3OH     + OH {+.85 O2} = .85 HCHO + .85 HO2 + .15 CH3O + H2O   : {%TrG} 6.38E-18*temp**2.*EXP(144./temp); {&1759}
<G4103a> CH3O2     + HO2      = CH3OOH + O2        : {%StTrG} 3.8E-13*EXP(780./temp)/(1.+1./498.*EXP(1160./temp)); {&1759}
<G4103b> CH3O2     + HO2      = HCHO + H2O + O2    : {%StTrG} 3.8E-13*EXP(780./temp)/(1.+498.*EXP(-1160./temp)); {&1759}
<G4104a> CH3O2     + NO       = CH3O + NO2         : {%StTrG} 2.3E-12*EXP(360./temp)*(1.-beta_CH3NO3); {&1759, 3177, 3164}
<G4104b> CH3O2     + NO       = CH3NO3             : {%StTrG} 2.3E-12*EXP(360./temp)*beta_CH3NO3; {&1759, 3177, 3164} // Methyl nitrate yield according to \citet{2130} but reduced by a factor of 10 according
to the upper limit derived from measurements by \citet{2048}.
<G4105>  CH3O2     + NO3      = CH3O + NO2 + O2    : {%TrG} 1.2E-12; {&1759}
<G4106a> CH3O2               = CH3O + .5 O2               : {%StTrG} 7.4E-13*EXP(-520./temp)*R02*2.; {&1759}
<G4106b> CH3O2               = .5 HCHO + .5 CH3OH + .5 O2  : {%StTrG} (k_CH3O2-7.4E-13*EXP(-520./temp))*R02*2.; {&1759}
<G4107>  CH3OOH    + OH       = .6 CH3O2 + .4 HCHO + .4 OH + H2O : {%StTrG} k_CH3OOH_OH; {&1207}
<G4108>  HCHO      + OH       = CO + H2O + HO2     : {%StTrG} 9.52E-18*EXP(2.03*LOG(temp)+636./temp); {&1634}
<G4109>  HCHO      + NO3      = HNO3 + CO + HO2    : {%TrG} 3.4E-13*EXP(-1900./temp); {&2626}
<G4110>  CO        + OH       = H + CO2 {+ 103. kJmol} : {%UpStTrG} (1.57E-13+cair*3.54E-33); {&1628}
<G4111>  HCOOH     + OH {+O2} = CO2 + HO2 + H2O    : {%TrG} 2.94E-14*exp(786./temp)+9.85E-13*EXP(-1036./temp); {&3038}
<G4112>  CO        + O3P {+M} = CO2 {+ 516. kJmol} : {%UpStG} 6.60E-33*EXP(-1103./temp); {&2615}
<G4113>  CH4       + O3P {+O2}= .51 CH3 + .51 OH + .49 CH3O + .49 H {+ 438. kJmol} : {%UpStG} 6.03E-18*temp**(2.17)*EXP(-3619./temp); {&2615, 3059, 3060}
<G4114>  CH3O2     + NO2      = CH3O2NO2           : {%StTrG} k_NO2_CH3O2; {&2626}
<G4115>  CH3O2NO2  {+ M}      = CH3O2 + NO2        : {%StTrG} k_NO2_CH3O2/(9.5E-29*EXP(11234./temp)); {&2626}
<G4116>  CH3O2NO2  + OH       = HCHO + NO3 + H2O   : {%StTrG} 3.00E-14 ; // Same value as for PAN + OH.
<G4117>  CH3NO3    + OH {+ O2}= H2O + HCHO + NO2   : {%StTrG} 4.0E-13*EXP(-845./temp); {&1759}
<G4118>  CH3O      {+ O2}     = HO2 + HCHO         : {%StTrG} 1.3E-14*exp(-663./temp)*c(ind_O2); {&3043}
<G4119a> CH3O      + NO2 {+ M}= CH3NO3             : {%StTrG} k_3rd_iupac(temp,cair,8.1E-29,4.5,2.1E-11,0.,0.44); {&1759}
<G4119b> CH3O      + NO2      = HCHO + HONO        : {%StTrG} 9.6E-12*EXP(-119.0./temp); {&1759}
<G4120a> CH3O      + NO       = CH3ONO             : {%StTrG} k_3rd_iupac(temp,cair,2.6E-29,2.8,3.3E-11,0.6,REAL(EXP(-temp/900.),SP)); {&1759}
<G4120b> CH3O      + NO       = HCHO + HNO         : {%StTrG} 2.3E-12*(temp/300.)**0.7; {&1759}
<G4121>  CH3O2     + O3       = CH3O + 2 O2        : {%StTrG} 2.9E-16*exp(-1000./temp); {&2626}
<G4122>  CH3ONO    + OH {+ O2}= H2O + HCHO + NO    : {%StTrG} 1.E-10*exp(-1764./temp); {&3044}
<G4123>  HCHO      + HO2      = HOCH2O2            : {%StTrG} 9.7E-15*EXP(625./temp); {&1759}
<G4124>  HOCH2O2             = HCHO + HO2         : {%StTrG} 2.4E12*EXP(-7000./temp); {&1759}
<G4125>  HOCH2O2   + HO2      = .5 HOCH2OOH + .5 HCOOH + .2 OH + .2 HO2 + .3 H2O + .8 O2 : {%StTrG} 5.6E-15*EXP(2300./temp); {&1759}
<G4126>  HOCH2O2   + NO {+ O2}= NO2 + HO2 + HCOOH  : {%StTrG} 0.7275*2.3E-12*EXP(360./temp); {&1759} // Same as for G4104 but scaled to match the recommeded value at 298K.
<G4127>  HOCH2O2   + NO3      = NO2 + HO2 + HCOOH  : {%StTrG} 1.2E-12;  // Same as for CH3O2 + NO3 in G4105.
<G4129a> HOCH2O2             = HCOOH + HO2                : {%StTrG} (k_CH3O2*5.5E-12)**0.5*R02*2.; {&1759}
<G4129b> HOCH2O2             = .5 HCOOH + .5 HOCH2OH + .5 O2 : {%StTrG} (k_CH3O2*5.7E-14*EXP(750./temp))**0.5*R02*2.; {&1759}
<G4130a> HOCH2OOH  + OH       = HOCH2O2 + H2O      : {%StTrG} 0.6*k_CH3OOH_OH; {&3030} // SAR for H-abstraction by OH.
<G4130b> HOCH2OOH  + OH       = HCOOH + H2O + OH   : {%StTrG} k_rohro + k_s*f_sooh*f_soh; {&3030} // SAR for H-abstraction by OH.
<G4132>  HOCH2OH   + OH {+ O2}= HO2 + HCOOH + H2O  : {%StTrG} k_rohro + 2.*k_s*f_soh*f_soh; {&3030} // SAR for H-abstraction by OH.
<G4133>  CH3O2     + OH       = CH3O + HO2         : {%StTrG} 1.4E-10; {&3042} // Lower limit of the rate constant. Products uncertain but \chem{CH_3OH} can be excluded because of a likely high energy
barrier (L.\ Vereecken, pers. comm.). \chem{CH_2OO} production cannot be excluded.
<G4134>  CH2OO     {+ O2}     = CO + HO2 + OH      : {%StTrG} 1.12E+14*EXP(-10000/temp); // Estimate based on the decomposition lifetime of 3 s \citep{3047} and a 20 kcal/mol energy barrier \citep{3040}.
<G4135>  CH2OO     + H2O      = HOCH2OOH           : {%StTrG} k_CH2OO_NO2*3.6E-6; {&3048} // Rate constant for \chem{CH_2OO + NO_2} (G4138) multiplied by the factor from \citet{3048}.
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<G4136>  CH2OO    + H2OH2O   = HOCH2OOH + H2O     : {%StTrG} 5.2E-12; {&3173, 3174} // Average of two measurements.
<G4137>  CH2OO    + NO       = HCHO + NO2         : {%StTrG} 6.E-14; {&3041} // Upper limit.
<G4138>  CH2OO    + NO2      = HCHO + NO3         : {%StTrG} k_CH2OO_NO2; {&3041, 3049} // Average of 7.E-12 and 1.5E-12.
<G4140>  CH2OO    + CO       = HCHO + CO2         : {%StTrG} 3.6E-14; {&3039}
<G4141>  CH2OO    + HCOOH    = 2 HCOOH            : {%StTrG} 1.E-10; {&3051} // \chem{HOOCH_2OCHO} forms and then decomposes to formic anhydride \citep{2071} which hydrolyses in the humid atmosphere
\citep{3045}.
<G4142>  CH2OO    + HCHO     = 2 LCARBON          : {%StTrG} 1.7E-12; {&3049} // High-pressure limit.
<G4143>  CH2OO    + CH3OH    = 2 LCARBON          : {%StTrG} 5.E-12; {&3039} // Generic estimate for reaction with alcohols.
<G4144>  CH2OO    + CH3O2    = 2 LCARBON          : {%StTrG} 5.E-12; {&3039} // Generic estimate for reaction with \chem{RO_2}.
<G4145>  CH2OO    + HO2      = LCARBON            : {%StTrG} 5.E-12; {&3039}
<G4146>  CH2OO    + O3       = HCHO + 2 O2        : {%StTrG} 1.E-12; {&3053}
<G4147>  CH2OO    + CH2OO    = 2 HCHO + O2        : {%StTrG} 6.E-11; {&3054}
<G4148>  HOCH2O2  + NO2      = HOCH2O2NO2         : {%StTrG} k_NO2_CH3O2; {&2626}
<G4149>  HOCH2O2NO2 {+ M}    = HOCH2O2 + NO2      : {%StTrG} k_NO2_CH3O2/(9.5E-29*EXP(11234./temp)); {&2626, 3055} // \citet{3055} estimated a decomposition rate equal to that of \chem{CH_3O_2NO_2}.
<G4150>  HOCH2O2NO2 + OH     = HCOOH + NO3 + H2O  : {%StTrG} 9.5OE-13*EXP(-650./temp)*f_soh; // Value for \chem{CH_3O_2NO_2} + OH, H-abstraction enhanced by the HO-group by f\_soh.
<G4151>  CH3      + O2 {+ M} = CH3O2              : {%StTrG} k_3rd_iupac(temp,cair,7.0E-31,3.,1.8E-12,-1.1,0.33); {&1759}
<G4152>  CH3      + O3       = .956 HCHO + .956 H + .044 CH3O + O2 : {%StTrG} 5.1E-12*exp(-210./temp); {&3056, 3057}
<G4153>  CH3      + O3P      = .83 HCHO + .83 H + .17 CO + .17 H2 + .17 H : {%StTrG} 1.3E-10; {&1759}
<G4154>  CH3O     + O3       = CH3O2 + O2         : {%StTrG} 2.53E-14; {&3056} // Products assumed to be \chem{CH_3O_2 + O_2} (could also be \chem{HCHO + O_2 + OH}).
<G4155>  CH3O     + O3P      = .75 CH3 + .75 O2 + .25 HCHO + .25 OH  : {%StTrG} 2.5E-11; {&3037}
<G4156>  CH3O2    + O3P      = CH3O + O2          : {%StTrG} 4.3E-11; {&3061}
<G4157>  HCHO     + O3P      = .7 OH + .7 CO + .3 H + .3 CO2 + HO2 : {%StTrG} 3.E-11*EXP(-1600./temp); {&2626}
<G4158>  CH2OOA             = .37 CH2OO + .47 CO + .47 H2O + .16 HO2 + .16 CO + .16 OH : {%TrG} KDEC; {&1759}
<G4159>  HCN      + OH       = H2O + CN           : {%TrG} k_3rd(temp,cair,4.28E-33,1.0,REAL(4.25E-13*EXP(-1150./temp),SP),1.0,0.8); {&3191}
<G4160a> HCN      + O1D      = O3P + HCN          : {%TrG} 1.08E-10*EXP(105./temp)*0.15*EXP(200/temp); {&3197}
<G4160b> HCN      + O1D      = H + NCO            : {%TrG} 1.08E-10*EXP(105./temp)*0.68/2.; {&3197} // Half of the H-yield is attributed to fast secondary chemistry.
<G4160c> HCN      + O1D      = OH + CN            : {%TrG} 1.08E-10*EXP(105./temp)*(1.-(0.68/2.+0.15*EXP(200/temp))); {&3197} // The NH + CO channel is also significant but neglected here.
<G4161>  HCN      + O3P      = H + NCO            : {%TrG} 1.0E-11*EXP(-4000./temp); {&2626} // No studies below 450 K and only the major channel is considered.
<G4162>  CN       + O2       = NCO + O3P          : {%TrG} 1.2E-11*EXP(210./temp)*0.75; {&3037}
<G4163>  CN       + O2       = CO +  NO           : {%TrG} 1.2E-11*EXP(210./temp)*0.25; {&3037}
<G4164>  NCO      + O2       = CO2 + NO           : {%TrG} 7.E-15; {&3198} // Upper limit. Dominant pathway under atmospheric conditions.
<G4200>  C2H6     + OH       = C2H5O2 + H2O                    : {%TrG} 1.49E-17*temp*temp*EXP(-499./temp); {&1759}
<G4201>  C2H4     + O3       = HCHO + CH2OOA                   : {%TrG} 9.1E-15*EXP(-2580./temp); {&1759} // The product distribution is from \citet{2419}, after substitution of the energized
Criegee intermediate, \chem{CH_2OO}, by its decomposition products and reaction of the stabilized CI with the water dimer.
<G4202>  C2H4     + OH {+O2} = HOCH2CH2O2              : {%TrG} k_3rd_iupac(temp,cair,8.6E-29,3.1,9.E-12,0.85,0.48); {&1759, 2419}
<G4203>  C2H5O2   + HO2      = C2H5OOH                 : {%TrG} 7.5E-13*EXP(700./temp); {&2626}
<G4204a> C2H5O2   + NO       = CH3CHO + HO2 + NO2      : {%TrG} 2.55E-12*EXP(380./temp)*(1.-beta_C2H5NO3); {&1759, 3170}
<G4204b> C2H5O2   + NO       = C2H5NO3                 : {%TrG} 2.55E-12*EXP(380./temp)*beta_C2H5NO3; {&1759, 3170}
<G4205>  C2H5O2   + NO3      = CH3CHO + HO2 + NO2      : {%TrG} 2.3E-12; {&1207}
<G4206>  C2H5O2             = .8 CH3CHO + .6 HO2 + .2 C2H5OH  : {%TrG} 2.*(7.6E-14*k_CH3O2)**(.5)*RO2; {&3031, 1759}
<G4207a> C2H5OOH + OH        = C2H5O2 + H2O            : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G4207b> C2H5OOH + OH        = CH3CHO + OH             : {%TrG} k_s*f_sooh; {&3031}
<G4208a> CH3CHO + OH         = CH3CO + H2O             : {%TrG} 4.4E-12*EXP(365./temp)*0.95; {&1759}
<G4208b> CH3CHO + OH         = HCOCH2O2 + H2O          : {%TrG} 4.4E-12*EXP(365./temp)*0.05; {&1759}
<G4209>  CH3CHO  + NO3       = CH3CO + HNO3            : {%TrG} KNO3AL; {&2419}
<G4210>  CH3CO2H + OH {+O2}= CH3 + CO2 + H2O           : {%TrG} 4.0E-14*EXP(850./temp); {&1759} // Only major channel considered as the end products are essentially the same.
<G4211a> CH3CO3 + HO2        = OH + CH3 + CO2          : {%TrG} 5.2OE-13*EXP(980./temp)*1.507*0.61; {&3156}
<G4211b> CH3CO3 + HO2        = CH3CO3H                 : {%TrG} 5.2OE-13*EXP(980./temp)*1.507*0.23; {&3156}
<G4211c> CH3CO3 + HO2        = CH3CO2H + O3            : {%TrG} 5.2OE-13*EXP(980./temp)*1.507*0.16; {&3156}
<G4212>  CH3CO3  + NO {+O2}= CH3 + CO2 + NO2           : {%TrG} 8.1E-12*EXP(270./temp); {&1613}
<G4213>  CH3CO3  + NO2       = PAN                     : {%TrG} k_CH3CO3_NO2; {&2626} // The rate coefficient is: \code{k_CH3CO3_NO2} = \code{k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6)}.
<G4214>  CH3CO3  + NO3       = CH3 + NO2 + CO2         : {%TrG} 4.E-12; {&1617}
<G4217a> CH3CO3              = CH3 + CO2               : {%TrG} k1_RO2RCO3*0.9; {&3031}
<G4217b> CH3CO3              = CH3CO2H                 : {%TrG} k1_RO2RCO3*0.1; {&3031}
<G4218>  CH3CO3H + OH        = CH3CO3 + H2O            : {%TrG} 0.6*k_CH3OOH_OH; {&2419} // The rate coefficient is the same as for the \kpp{CH3} channel in G4107 (\kpp{CH3OOH}+\kpp{OH}).
<G4220>  PAN      + OH       = HCHO + CO + NO2 + H2O   : {%TrG} 3.00E-14; {&2419}
<G4221>  PAN      {+M}       = CH3CO3 + NO2            : {%TrG} k_PAN_M; {&2626} // The rate coefficient is \code{k_PAN_M} = \code{k_CH3CO3_NO2/9.E-29*EXP(-14000./temp)}, i.e.\ the rate
coefficient is defined as backward reaction divided by equilibrium constant.
<G4222a> C2H2       + OH     = GLYOX + OH              : {%TrG} k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,2.,0.6)*.71; {&2626, 3176}
<G4222b> C2H2       + OH     = HCOOH + CO + HO2        : {%TrG} k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,2.,0.6)*(1.-.71); {&2626, 3176}
<G4223a> HOCH2CHO   + OH     = HOCH2CO + H2O           : {%TrG} 8.00E-12*0.80; {&1759}
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<G42023b> HOCH2CH0   + OH   = HOCHCH0 + H2O                          : {%TrG} 8.00E-12*0.20; {&1759}
<G42024a> HOCH2CO    + O2   = HOCH2CO3                               : {%TrG} 5.1E-12*(1.-1./(1+1.85E-18*cair)); {&1759, 3163} // Rate constant is the high-pressure limit as recommended by \citet{1759}.
<G42024b> HOCH2CO    + O2   = OH + HCH0 + CO2                        : {%TrG} 5.1E-12*1./(1+1.85E-18*cair); {&1759, 3163} // Rate constant is the high-pressure limit as recommended by \citet{1759}.
<G42025>  HOCHCH0 {+ O2}    = GLYOX + HO2                            : {%TrG} KDEC; {&3031}
<G42026>  HOCH2CH0   + NO3  = HOCH2CO + HNO3                         : {%TrG} KNO3AL; {&2419}
<G42027a> HOCH2CO3          = HCH0 + CO2 + HO2                       : {%TrG} k1_RO2RCO3*0.9; {&3031}
<G42027b> HOCH2CO3          = HOCH2CO2H                              : {%TrG} k1_RO2RCO3*0.1; {&3031}
<G42028a> HOCH2CO3 + HO2    = HCH0 + HO2 + OH + CO2                  : {%TrG} KAPHO2*rco3_oh; {&3031, 3156}
<G42028b> HOCH2CO3 + HO2    = HOCH2CO3H                              : {%TrG} KAPHO2*rco3_ooh; {&3031, 3156}
<G42028c> HOCH2CO3 + HO2    = HOCH2CO2H + O3                         : {%TrG} KAPHO2*rco3_o3; {&3031, 3156}
<G42029>  HOCH2CO3   + NO   = NO2 + HO2 + HCH0  + CO2                : {%TrG} KAPNO; {&2419}
<G42030>  HOCH2CO3   + NO2  = PHAN                                   : {%TrG} k_CH3CO3_NO2; {&2419}
<G42031>  HOCH2CO3   + NO3  = NO2 + HO2 + HCH0  + CO2                : {%TrG} KRO2NO3*1.60; {&2419}
<G42032>  HOCH2CO2H + OH    = .09 HCH0 + .09 CO2 + .91 HCOCO2H + HO2 + H2O : {%TrG} k_co2h+k_s*f_soh*f_co2h; {&3031}
<G42033a> HOCH2CO3H + OH    = HOCH2CO3 + H2O                         : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G42033b> HOCH2CO3H + OH    = HCOCO3H + HO2                          : {%TrG} k_s*f_soh*f_co2h; {&3031}
<G42034>  PHAN              = HOCH2CO3 + NO2                         : {%TrG} k_PAN_M; {&2419}
<G42035>  PHAN       + OH   = HCH0 + CO + NO2 + H2O                  : {%TrG} k_s*f_soh*f_cpan+k_rohro; {&3031}
<G42036>  GLYOX      + OH   = HCOCO + H2O                            : {%TrG} 3.1E-12*EXP(340./temp); {&1759, 3150, 3169}
<G42037>  GLYOX      + NO3  = HCOCO + HNO3                           : {%TrG} KNO3AL; {&2419}
<G42038a> HCOCO             = CO + CO + HO2                          : {%TrG} 7.E11*EXP(-3160./temp)+5.E-12*c(ind_02); {&3150, 3169, 2419}
<G42037b> HCOCO      {+ O2} = HCOCO3                                 : {%TrG} 5.E-12*c(ind_02)*3.2*exp(-550./temp); {&3169, 2419}
<G42037c> HCOCO      {+ O2} = OH + CO + CO2                          : {%TrG} 5.E-12*c(ind_02)*(1.-3.2*exp(-550./temp)); {&3169, 2419}
<G42039a> HCOCO3            = CO + HO2 + CO2                         : {%TrG} k1_RO2RCO3*0.9; {&3031}
<G42039b> HCOCO3            = HCOCO2H                                : {%TrG} k1_RO2RCO3*0.1; {&3031}
<G42040>  HCOCO3     + HO2  = HO2 + CO + CO2 + OH                    : {%TrG} KAPHO2; {&3157, 3031}
<G42041>  HCOCO3     + NO   = HO2 + CO + NO2 + CO2                   : {%TrG} KAPNO; {&2419}
<G42042>  HCOCO3     + NO3  = HO2 + CO + NO2 + CO2                   : {%TrG} KRO2NO3*1.60; {&2419}
<G42043>  HCOCO3     + NO2  = HO2 + CO + NO3 + CO2                   : {%TrG} k_CH3CO3_NO2; {&3150, 3031}
<G42044>  HCOCO2H    + OH   = CO + HO2 + CO2 + H2O                   : {%TrG} k_co2h+k_t*f_o*f_co2h; {&3031}
<G42045a> HCOCO3H    + OH   = HCOCO3 + H2O                           : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G42045b> HCOCO3H    + OH   = CO + CO2 + H2O + OH                    : {%TrG} k_t*f_o*f_co2h; {&3031}
<G42046>  HOCH2CH2O2        = .6 HOCH2CH2O + .2 HOCH2CH0 + .2 ETHGLY   : {%TrG} 2.*(7.8E-14*EXP(1000./temp)*k_CH3O2)**(.5)*RO2; {&1759, 2419}
<G42047>  HOCH2CH2O2 + NO   = .25 HO2 + .5 HCH0 + .75 HOCH2CH2O + NO2  : {%TrG} KRO2NO*(1.-alpha_AN(3,1,0,0,0,temp,cair)); {&2419} // \citet{2425} estimated that about 25\% of the \kpp{HOCH2CH2O} in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 \kpp{HCH0} + \kpp{HO2}.
<G42048>  HOCH2CH2O2 + NO   = ETHOHNO3                               : {%TrG} KRO2NO*alpha_AN(3,1,0,0,0,temp,cair); {&3031}
<G42049a> HOCH2CH2O2 + HO2  = HYETHO2H                               : {%TrG} 1.53E-13*EXP(1300./temp)*(1.-rchohch2o2_oh); {&2419}
<G42049b> HOCH2CH2O2 + HO2  = HOCH2CH2O + OH                         : {%TrG} 1.53E-13*EXP(1300./temp)*rchohch2o2_oh; {&2419}
<G42050>  ETHOHNO3   + OH   = .93 NO3CH2CH0 + .93 HO2 + .07 HOCH2CH0 + .07 NO2 + H2O : {%TrG} k_s*(f_soh*f_ch2ono2+f_ono2*f_pch2oh)+k_rohro; {&3031}
<G42051a> HYETHO2H   + OH   = HOCH2CH2O2 + H2O                       : {%TrG} 0.6*k_CH3OOH_OH; {&2419} // Same as for the \chem{CH_3O_2} channel in G4107: \kpp{CH3OOH}+\kpp{OH}.
<G42051b> HYETHO2H   + OH   = HOCH2CH0 + OH + H2O                    : {%TrG} k_s*f_sooh*f_pch2oh; {&3031}
<G42051c> HYETHO2H   + OH   = HOOCH2CH0 + HO2 + H2O                  : {%TrG} k_s*f_soh*f_pch2oh+k_rohro; {&3031}
<G42052a> HOCH2CH2O {+ O2}  = HO2 + HOCH2CH0                         : {%TrG} 6.00E-14*EXP(-550./temp)*C(ind_02); {&2419}
<G42052b> HOCH2CH2O         = HO2 + HCH0 + HCH0                      : {%TrG} 9.50E13*EXP(-5988./temp); {&2419}
<G42053>  ETHGLY + OH       = HOCH2CH0 + HO2 + H2O                   : {%TrG} 2*k_s*f_soh*f_pch2oh+2*k_rohro; {&3031}
<G42054>  HCOCH2O2          =  .6 HCH0 + .6 CO + .6 HO2 + .2 GLYOX + .2 HOCH2CH0 : {%TrG} k1_RO2pORO2; {&3031}
<G42055a> HCOCH2O2 + HO2    =  HOOCH2CH0                             : {%TrG} KRO2HO2(2)*rcoch2o2_ooh; {&3031}
<G42055b> HCOCH2O2 + HO2    =  HCH0 + CO + HO2 + OH                  : {%TrG} KRO2HO2(2)*rcoch2o2_oh; {&3031}
<G42056a> HCOCH2O2 + NO     =  NO2 + HCH0 + CO + HO2                 : {%TrG} KRO2NO*(1.-alpha_AN(3,1,1,0,0,temp,cair)); {&3031}
<G42056b> HCOCH2O2 + NO     =  NO3CH2CH0                             : {%TrG} KRO2NO*alpha_AN(3,1,1,0,0,temp,cair); {&3031}
<G42057>  HCOCH2O2 + NO3    =  HCH0 + CO + HO2 + NO2                 : {%TrG} KRO2NO3; {&3031}
<G42058a> HOOCH2CH0 + OH    = HCOCH2O2                               : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G42058b> HOOCH2CH0 + OH    =  HCH0 + CO + OH                        : {%TrG} .8*8.E-12; {&3031} // The aldehydic H is assumed to be like the analogous H of \kpp{HOCH2CH0}.
<G42058c> HOOCH2CH0 + OH    = GLYOX + OH                             : {%TrG} k_s*f_sooh*f_cho; {&3031}
<G42059>  HOOCH2CH0 + NO3   = OH + HCH0 + CO + HNO3                  : {%TrG} KNO3AL; {&2419}
<G42060>  HOOCH2CO3 + NO    = NO2 + OH + HCH0 + CO2                  : {%TrG} KAPNO; {&3031}
<G42061>  HOOCH2CO3 + NO3   = NO2 + OH + HCH0 + CO2                  : {%TrG} KRO2NO3*1.60; {&3031}
<G42062a> HOOCH2CO3 + HO2   = 2 OH + HCH0 + CO2                      : {%TrG} KAPHO2*rco3_oh; {&3031}
<G42062b> HOOCH2CO3 + HO2   = HOOCH2CO3H                             : {%TrG} KAPHO2*rco3_ooh; {&3031}
<G42062c> HOOCH2CO3 + HO2   = HOOCH2CO2H + O3                        : {%TrG} KAPHO2*rco3_o3; {&3031}
<G42063a> HOOCH2CO3         = OH + HCH0 + CO2                        : {%TrG} k1_RO2RCO3*0.9; {&3031}
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<G42063b> HOOCH2CO3          = HOOCH2CO2H                                : {%TrG} k1_RO2RCO3*0.1; {&3031}
<G42064a> HOOCH2CO3H + OH    = HOOCH2CO3 + H2O                           : {%TrG} 2.*0.6*k_CH3OOH_OH; {&3031}
<G42064b> HOOCH2CO3H + OH    = HCOCO3H + OH + H2O                        : {%TrG} k_s*f_sooh*f_co2h; {&3031}
<G42065>  HOOCH2CO2H + OH    = HCOCO2H + OH + H2O                        : {%TrG} k_s*f_sooh*f_co2h+k_co2h; {&3031}
<G42066>  CH2CO      + OH    = .6 HCHO + .6 HO2 + .6 CO + .4 HOOCH2CO2H  : {%TrG} 2.8E-12*exp(510./temp); {&3037, 3031}
<G42067a> CH3CH0H00H + OH    = CH3CO2H + OH                              : {%TrG} (k_t*f_tooh*f_toh + k_rohro); {&3031}
<G42067b> CH3CH0H00H + OH    = CH3CH0HO2                                 : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G42068>  CH3CH0H02          = CH3CH0 + HO2                              : {%TrG} 3.4E12*EXP(-1250./(1.98*temp)); {&3153, 3031}
<G42069>  CH3CH0 + HO2       = CH3CH0H02                                 : {%TrG} 3.4E12*EXP(-1250./(1.98*temp))/(6.34E26*EXP(-14700./(1.98*temp))); {&3153, 3031}
<G42070>  CH3CH0H02 + HO2    = .5 CH3CH0H00H + .3 CH3CO2H + .2 CH3 + .2 HCOOH + .2 OH   : {%TrG} 5.6E-15*EXP(2300./temp); {&3031}
<G42071>  CH3CH0H02          = CH3 + HCOOH + OH                          : {%TrG} k1_RO2s0RO2; {&3031}
<G42072>  CH3CH0H02 + NO     = CH3 + HCOOH + OH + NO2                    : {%TrG} KRO2NO; {&3031}
<G42073>  C2H5NO3 + OH       = CH3CH0 + H2O + NO2                        : {%TrG} 6.7E-13*EXP(-395./temp); {&1759}
<G42074a> NO3CH2CH0 + OH     = GLYOX + NO2 + H2O                         : {%TrG} k_s*f_ch2ono2*f_cho; {&3159, 3031} // Factor of 3 to match the estimate of k = 1.E-11 molec/cm3/s by \citet{3159}.
<G42074b> NO3CH2CH0 + OH     = NO3CH2CO3 + H2O                           : {%TrG} k_t*f_o*f_ch2ono2*3.; {&3159, 3031} // Factor of 3 to match the estimate of k = 1.E-11 molec/cm3/s by \citet{3159}.
<G42075>  NO3CH2CO3 + HO2    = HCHO + NO2 + CO2 + OH                     : {%TrG} KAPH02; {&2419} // \chem{NO_3CH_2CO_2H} and \chem{NO_3CH_2CO_3H} neglected.
<G42076>  NO3CH2CO3 + NO     = HCHO + NO2 + CO2 + NO2                    : {%TrG} KAPNO; {&2419}
<G42077>  NO3CH2CO3 + NO2    = NO3CH2PAN                                 : {%TrG} k_CH3CO3_NO2; {&2419}
<G42078>  NO3CH2CO3          = HCHO + NO2 + CO2                          : {%TrG} k1_RO2RCO3; {&2419} // \chem{NO_3CH_2CO_2H} neglected.
<G42079>  NO3CH2PAN {+ M}    = NO3CH2CO3 + NO2                           : {%TrG} k_PAN_M; {&2419}
<G42080>  C2H5O2 + NO2 {+ M}= C2H5O2NO2                                  : {%StTrG} k_3rd_iupac(temp,cair,1.3E-29,6.2,8.8E-12,0.0,0.31); {&1759}
<G42081>  C2H5O2NO2 {+ M}    = C2H5O2 + NO2                              : {%StTrG} k_3rd_iupac(temp,cair,REAL(4.8E-4*EXP(-9285./temp),SP),0.0,REAL(8.8E15*EXP(-10440./temp),SP),0.0,0.31); {&1759}
<G42082>  C2H5O2NO2 + OH     = CH3CH0 + NO3 + H2O                        : {%StTrG} 9.5OE-13*EXP(-650./temp); {&3031} // Same rate constant as for PAN + OH.
<G42083a> CH3CO      + O2    = CH3CO3                                    : {%TrG} 5.1E-12*(1. - 1./(1.+9.4E-18*cair)); {&1759, 3163} // Rate constant is the high-pressure limit as recommended by \citet{1759}.
<G42083b> CH3CO      + O2    = OH + HCHO + CO                            : {%TrG} 5.1E-12*1./(1.+9.4E-18*cair); {&1759, 3163} // Rate constant is the high-pressure limit as recommended by \citet{1759}.
<G42084>  C2H5OH + OH        = .95 C2H5O2 + .95 HO2 + .05 HOCH2CH2O2 + H2O : {%TrG} 3.0E-12*EXP(20./temp); {&3031, 1759}
<G42085a> CH3CN + OH         = NCCH2O2 + H2O                             : {%TrG} 8.1E-13*EXP(-1080./temp)*0.40; {&1759, 3212} // Uncertainties on the kinetics at pressures $<$ 0.1 bar.
<G42085b> CH3CN + OH         = OH + CH3CO + NO                           : {%TrG} 8.1E-13*EXP(-1080./temp)*(1.-0.40); {&1759, 3212} // Channel proposed by Hynes and Wine 1991, OH + HCHO + HOCN, could not be
confirmed by \cite{3212}. There is no alternative mechanism at the moment. Products assumed to be OH + CH3CO3 + NO
<G42086a> CH3CN + O1D        = O3P + CH3CN                               : {%TrG} 2.54E-10*EXP(-24./temp)*0.0269*EXP(137./temp); {&3197}
<G42086b> CH3CN + O1D        = 2 H + CO + HCN                            : {%TrG} 2.54E-10*EXP(-24./temp)*0.16; {&3197} // Assuming HCN is from channel 2h, HCO + H + HCN. HCO is replaced by H + CO.
<G42086c> CH3CN + O1D        = .5 CH3 + .5 NCO + .5 NCCH2O2 + .5 OH      : {%TrG} 2.54E-10*EXP(-24./temp)*(1.-(0.16+0.0269*EXP(137./temp))); {&3197} // Assuming exothermic channels 2b and 2d are equally
important.
<G42087>  NCCH2O2 + NO       = HCN + CO2 + HO2 + NO2                     : {%TrG} KRO2NO; // HCOCN is produced but replaced here by its likely oxidation products (HCN + \chem{CO_2}) as studied by \cite{3212}.
The rate constant for a typical \chem{RO_2} + NO reaction is used.
<G42088>  NCCH2O2 + HO2      = HCN + CO2 + H2O                           : {%TrG} KRO2HO2(2); // \chem{NCCH_2OOH} is produced but replaced here by its likely oxidation products (HCN + \chem{CO_2}) as studied
by \cite{3212}. The rate constant for a typical \chem{RO_2} + \chem{HO_2} reaction is used.
<G42089a> CH2CH0H + OH       = HCOOH + OH + HCHO                         : {%TrG} k_CH2CH0H_OH_HCOOH; {&3031, 3179} // The minor channel with k=5.2E-12 is combined with the major one producing \chem{HCOOH}.
<G42089b> CH2CH0H + OH       = HOCH2CHO + HO2                            : {%TrG} k_CH2CH0H_OH_ALD; {&3031, 3179}
<G42090>  CH2CH0H + HCOOH    = CH3CH0 + HCOOH                            : {%TrG} k_CH2CH0H_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G42091>  CH3CH0 + HCOOH     = CH2CH0H + HCOOH                           : {%TrG} k_ALD_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G43000a> C3H8         + OH  = IC3H7O2 + H2O    : {%TrG} k_s; {&3031}
<G43000b> C3H8         + OH  = NC3H7O2 + H2O    : {%TrG} 2.*k_p; {&3031}
<G43001a> C3H6         + O3  = HCHO + .16 CH3CH0H00H + .50 OH + .50 HCOCH2O2 + .05 CH2CO + .09 CH3OH + .09 CO + .2 CH4 + .2 CO2 : {%TrG} 5.5E-15*EXP(-1880./temp)*.57; {&1759} // Branching ratios according to
\citet{3200}.
<G43001b> C3H6         + O3  = CH3CH0 + CH2OOA                                                                    : {%TrG} 5.5E-15*EXP(-1880./temp)*.43; {&1759} // Branching ratios according to \citet{3200}.
<G43002>  C3H6 {+M}    + OH  = HYPROPO2                                : {%TrG} k_3rd_iupac(temp,cair,8.6E-27,3.5,3.E-11,1.,0.5); {&1759, 2419}
<G43003>  C3H6         + NO3 = PRONO3BO2                               : {%TrG} 4.6E-13*EXP(-1155./temp); {&1207}
<G43004>  IC3H7O2      + HO2 = IC3H7OOH                                : {%TrG} 1.9E-13*EXP(1300./temp); {&964} // The value for the generic \chem{RO_2} + \chem{HO_2} reaction from \citet{964} is used here.
<G43005a> IC3H7O2      + NO  = CH3COCH3 + HO2 + NO2                    : {%TrG} 2.7E-12*EXP(360./temp)*(1.-alpha_AN(3,2,0,0,0,temp,cair)); {&1207}
<G43005b> IC3H7O2      + NO  = IC3H7NO3                                : {%TrG} 2.7E-12*EXP(360./temp)*alpha_AN(3,2,0,0,0,temp,cair); {&1207}
<G43006>  IC3H7O2            = .8 CH3COCH3 + .2 IPROPOL + .6 HO2       : {%TrG} 2.*(1.6E-12*EXP(-2200./temp)*k_CH3O2)**(.5)*RO2; {&2419, 1759}
<G43007a> IC3H7OOH     + OH  = IC3H7O2 + H2O                           : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G43007b> IC3H7OOH     + OH  = CH3COCH3 + H2O + OH                     : {%TrG} k_t*f_tooh; {&3031}
<G43008>  NC3H7O2      + HO2 = NC3H7OOH                                : {%TrG} 1.9E-13*EXP(1300./temp); {&964} // The value for the generic \chem{RO_2} + \chem{HO_2} reaction from \citet{964} is used here.
<G43009a> NC3H7O2      + NO  = C2H5CHO + HO2 + NO2                     : {%TrG} 2.7E-12*EXP(360./temp)*(1.-alpha_AN(3,1,0,0,0,temp,cair)); {&1207}
<G43009b> NC3H7O2      + NO  = NC3H7NO3                                : {%TrG} 2.7E-12*EXP(360./temp)*alpha_AN(3,1,0,0,0,temp,cair); {&1207}
<G43010>  NC3H7O2            = .8 CH3COCH3 + .2 NPROPOL + .6 HO2       : {%TrG} 2.*(k_CH3O2*3.E-13)**(.5)*RO2; {&2419, 1759}
<G43011>  CH3COCH3     + OH  = CH3COCH2O2 + H2O                        : {%TrG} (8.8E-12*EXP(-1320./temp)+1.7E-14*EXP(423./temp)); {&1759} // Strong positive deviation of k below 240 K compared to the
expression recommended by JPL \citep{2626}.
<G43012a> CH3COCH2O2   + HO2 = HYPERACET                              : {%TrG} 8.6E-13*EXP(700./temp)*rcoch2o2_ooh; {&1613, 3031}
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<G43012b> CH3COCH2O2  + HO2 = OH + CH3CO + HCHO                      : {%TrG} 8.6E-13*EXP(700./temp)*rcoch2o2_oh; {&1613, 3031}
<G43013a> CH3COCH2O2  + NO  = CH3CO + HCHO + NO2                     : {%TrG} 2.9E-12*EXP(300./temp)*(1.-alpha_AN(4,1,1,0,0,temp,cair)); {&2626}
<G43013b> CH3COCH2O2  + NO  = NOA                                    : {%TrG} 2.9E-12*EXP(300./temp)*alpha_AN(4,1,1,0,0,temp,cair); {&2626}
<G43014>  CH3COCH2O2        = .3 CH3CO + .3 HCHO + .5 MGLYOX + .2 ACETOL : {%TrG} kl_RO2pOR02; {&3175}
<G43015a> HYPERACET   + OH  = CH3COCH2O2 + H2O                       : {%TrG} 0.6*k_CH3OOH_OH; // The same value as for G4107 (\kpp{CH3OOH} + \kpp{OH}) is used, multiplied by the branching ratio of the
\kpp{CH3O2} channel.
<G43015b> HYPERACET   + OH  = MGLYOX + OH + H2O                      : {%TrG} k_s*f_sooh*f_co; {&3031}
<G43016>  ACETOL      + OH  = MGLYOX + HO2 + H2O                     : {%TrG} 1.6E-12*EXP(305./temp); {&1759}
<G43017>  MGLYOX      + OH  = .4 CH3 + .6 CH3CO + 1.4 CO + H2O       : {%TrG} 1.9E-12*EXP(575./temp); {&3149, 1759}
<G43020>  IC3H7NO3    + OH  = CH3COCH3 + NO2                         : {%TrG} 6.2E-13*EXP(-230./temp); {&1207}
<G43021>  CH3COCH2O2  + NO3 = CH3CO + HCHO + NO2                     : {%TrG} KR02NO3; {&2419}
<G43022>  HYPROPO2          = CH3CHO + HCHO + HO2                    : {%TrG} kl_RO2s0R02; {&2419}
<G43023a> HYPROPO2    + HO2 = HYPROPO2H                              : {%TrG} KR02HO2(3)*(1.-rchohch2o2_oh); {&2419}
<G43023b> HYPROPO2    + HO2 = CH3CHO + HCHO + HO2 + OH               : {%TrG} KR02HO2(3)*rchohch2o2_oh; {&2419}
<G43024a> HYPROPO2    + NO  = CH3CHO + HCHO + HO2 + NO2              : {%TrG} KR02NO*(1.-alpha_AN(4,1,0,0,0,temp,cair)); {&2419}
<G43024b> HYPROPO2    + NO  = PROPOLNO3                              : {%TrG} KR02NO*alpha_AN(4,1,0,0,0,temp,cair); {&2419}
<G43025>  HYPROPO2    + NO3 = CH3CHO + HCHO + HO2 + NO2              : {%TrG} KR02NO3; {&2419}
<G43026a> HYPROPO2H   + OH  = HYPROPO2                               : {%TrG} 0.6*k_CH3OOH_OH; {&2419}
<G43026b> HYPROPO2H   + OH  = ACETOL + OH                            : {%TrG} (k_s*f_soh*f_pch2oh+k_t*f_tooh*f_pch2oh); {&3031}
<G43027>  PRONO3BO2   + HO2 = PR2O2HNO3                              : {%TrG} KR02HO2(3); {&2419}
<G43028>  PRONO3BO2   + NO  = NOA + HO2 + NO2                        : {%TrG} KR02NO; {&2419} // \alkylnitrateneglected\ (also not considered in MCM).
<G43029>  PRONO3BO2   + NO3 = NOA + HO2 + NO2                        : {%TrG} KR02NO3; {&2419}
<G43030a> PR2O2HNO3   + OH  = PRONO3BO2                              : {%TrG} 0.6*k_CH3OOH_OH; {&2419}
<G43030b> PR2O2HNO3   + OH  = NOA + OH                               : {%TrG} k_t*f_tooh*f_ch2ono2; {&3031}
<G43031>  MGLYOX      + NO3 = CH3CO + CO + HNO3                      : {%TrG} KNO3AL*2.4; {&2419}
<G43032>  NOA         + OH  = MGLYOX + NO2                           : {%TrG} (k_s*f_co*f_ono2+k_p*f_co); {&3031}
<G43033>  HOCH2COCHO  + OH  = .8609 HOCH2CO + .8609 CO + .1391 C33CO + .1391 HO2 : {%TrG} (1.9E-12*EXP(575./temp)+k_s*f_soh*f_co); {&3031}
<G43034>  HOCH2COCHO  + NO3 = HOCH2CO + CO + HNO3                    : {%TrG} KNO3AL*2.4; {&3031}
<G43035>  CH3CO2H     + OH  = CH3CO + H2O + CO2                      : {%TrG} 4.9E-14*EXP(276./temp); {&3154, 3031}
<G43036>  CH0CO2H2O         = .6 HCOCO + .6 HCHO + .2 C33CO + .2 HOCH2COCHO : {%TrG} kl_RO2pOR02; {&3031}
<G43037>  CH0CO2H2O2 + NO   = HCOCO + HCHO + NO2                     : {%TrG} KR02NO; {&3031} // \alkylnitrateneglected\ (also not considered in MCM).
<G43038a> CH0CO2H2O2 + HO2  = ALCOCH2OOH                             : {%TrG} KR02HO2(3)*rcoch2o2_ooh; {&3031}
<G43038b> CH0CO2H2O2 + HO2  = HCOCO + HCHO + OH                      : {%TrG} KR02HO2(3)*rcoch2o2_oh; {&3031}
<G43039>  CH0CO2H2O2 + NO3  = HCOCO + HCHO + NO2                     : {%TrG} KR02NO3; {&3031}
<G43040a> ALCOCH2OOH + OH   = HOOCH2CO3 + CO + H2O                   : {%TrG} k_t*f_co*f_o; {&3031} // Rate coefficient estimated with SAR \citep{3030}.
<G43040b> ALCOCH2OOH + OH   = C33CO + H2O + OH                       : {%TrG} k_s*f_sooh*f_co; {&3031} // Rate coefficient estimated with SAR \citep{3030}.
<G43040c> ALCOCH2OOH + OH   = CH0CO2H2O2 + H2O                       : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G43041>  ALCOCH2OOH + NO3  = HOOCH2CO3 + CO + HNO3                  : {%TrG} KNO3AL*2.4; {&3031}
<G43042>  HOCH2CO2CH2O2       = HCHO + HOCH2CO                       : {%TrG} kl_RO2pOR02; {&3031}
<G43043a> HOCH2CO2CH2O2 + HO2 = HOCH2CO2CH2OOH                       : {%TrG} KR02HO2(3)*rcoch2o2_ooh; {&3031}
<G43043b> HOCH2CO2CH2O2 + HO2 = HCHO + HOCH2CO + OH                  : {%TrG} KR02HO2(3)*rcoch2o2_oh; {&3031}
<G43044>  HOCH2CO2CH2O2 + NO  = HCHO + HOCH2CO + NO2                 : {%TrG} KR02NO; {&3031} // \alkylnitrateneglected
<G43045a> HOCH2CO2CH2OOH + OH = HOCH2CO2CHO + OH                     : {%TrG} k_s*f_sooh*f_co; {&3031}
<G43045b> HOCH2CO2CH2OOH + OH = HOCH2CO2CH2O2                        : {%TrG} .6*k_CH3OOH_OH; {&3031}
<G43045c> HOCH2CO2CH2OOH + OH = HCOCO2CH2OOH + HO2                   : {%TrG} 1.6OE-12*EXP(305./temp); {&3031} // Rate coefficient assumed to equal to the one of hydroxyacetone (ACETOL) for this channel.
<G43046>  CH3CHCO     + OH    = .72 CO + .72 CH3CHO + .72 HO2 + .21 CH3COCO2H + .07 CH3CHO + .07 HO2 + .07 CO2 : {%TrG} 7.6E-11; {&3155, 3031}
<G43047>  PROPOLNO3 + OH      = ACETOL + NO2                         : {%TrG} k_t*f_ono2*f_pch2oh+k_s*f_soh*f_ch2ono2; {&3031}
<G43048>  CH3COCH2O2  + NO2   = CH3COCH2O2NO2                        : {%TrG} 2.3E-12*EXP(300./temp); {&1613} // Using the high-pressure limit.
<G43049>  CH3COCH2O2NO2 {+ M}= CH3COCH2O2  + NO2                     : {%TrG} 1.9E16*EXP(-10830./temp); {&3166} // The pressure fall-off between 1000 and 100 mbar is only 3\% \citep{3165}.
<G43050>  CH3COCH2O2NO2 + OH = MGLYOX + NO3 + H2O                    : {%TrG} 9.50E-13*EXP(-650./temp)*f_co; {&3031} // Value for \chem{CH_3O_2NO_2} + OH, H-abstraction enhanced by the \chem{CH_3CO}-group
by f\_co.
<G43051a> NC3H7OOH    + OH  = NC3H7O2 + H2O                          : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G43051b> NC3H7OOH    + OH  = C2H5CHO + H2O + OH                     : {%TrG} k_s*f_sooh; {&3031}
<G43051c> NC3H7OOH    + OH  = C2H5CHO + HO2 + H2O                    : {%TrG} k_s*f_pch2oh; {&3031} // Products approximated with \kpp{C2H5CHO} + \kpp{HO2}.
<G43052>  C2H5CHO     + OH  = C2H5CO3 + H2O                          : {%TrG} 4.9E-12*EXP(405./temp); {&1759} // Only major H-abstraction channel considered.
<G43053>  C2H5CHO     + NO3 = C2H5CO3 + HNO3                         : {%TrG} 6.3E-15; {&1759}
<G43054a> C2H5CO3           = C2H5O2 + CO2                         : {%TrG} kl_RO2RCO3*0.9; {&3031}
<G43054b> C2H5CO3           = C2H5CO2H                             : {%TrG} kl_RO2RCO3*0.1; {&3031}
<G43055a> C2H5CO3 + HO2     = C2H5O2 + CO2 + OH                    : {%TrG} KAPHO2*rco3_oh; {&3031, 3156}
<G43055b> C2H5CO3 + HO2     = C2H5CO3H                             : {%TrG} KAPHO2*rco3_ooh; {&3031, 3156}
<G43055c> C2H5CO3 + HO2     = C2H5CO2H + O3                        : {%TrG} KAPHO2*rco3_o3; {&3031, 3156}
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<G43056>  C2H5CO3   + NO     = NO2 + C2H5O2 + CO2                    : {%TrG} KAPNO; {&2419}
<G43057>  C2H5CO3   + NO2    = PPN                                   : {%TrG} k_CH3CO3_NO2; {&2419}
<G43058>  PPN                = C2H5CO3 + NO2                         : {%TrG} k_PAN_M; {&2419}
<G43059>  C2H5CO2H   + OH    = CH3CHO + CO2 + H2O                    : {%TrG} k_co2h+k_p+k_s*f_co2h; {&3031} // Products approximated with the major end-product \kpp{CH3CHO}.
<G43060a> C2H5CO3H   + OH    = C2H5CO3 + H2O                         : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G43060b> C2H5CO3H   + OH    = CH3CHO + CO2 + H2O                    : {%TrG} k_s*f_co2h+k_p; {&3031} // Products approximated with the major end-product \kpp{CH3CHO}.
<G43061>  PPN        + OH    = CH3CHO + CO2 + NO2 + H2O              : {%TrG} k_s*f_cpan+k_p; {&3031} // Products approximated with the likely end-product \kpp{CH3CHO}.
<G43062>  CH3CO3H + OH       = CH3CO3 + H2O                          : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G43063a> CH3CO3 + HO2       = CH3CO + CO2 + OH                      : {%TrG} KAPHO2*rco3_oh; {&3031}
<G43063b> CH3CO3 + HO2       = CH3CO3H                               : {%TrG} KAPHO2*(rco3_ooh+rco3_o3); {&3031}
<G43064>  CH3CO3 + NO        = CH3CO + CO2 + NO2                     : {%TrG} KAPNO; {&3031}
<G43065>  CH3CO3 + NO2       = CH3CO + CO2 + NO3                     : {%TrG} k_CH3CO3_NO2; {&3031} // As for \kpp{HCOCO3}.
<G43066>  CH3CO3 + NO3       = CH3CO3 + CO2 + NO2                    : {%TrG} KRO2NO3*1.74; {&3031}
<G43067>  CH3CO3             = CH3CO3 + CO2                          : {%TrG} k1_RO2RC03; {&3031}
<G43068>  C33CO   + OH       = 3 CO + HO2                            : {%TrG} 2.*k_t*f_co*f_o; {&3031}
<G43069>  IPROPOL + OH       = CH3COCH3 + HO2 + H2O                  : {%TrG} 2.6E-12*EXP(200./temp); {&1759}
<G43070a> NPROPOL + OH       = C2H5CHO + HO2 + H2O                   : {%TrG} 4.6E-12*EXP(70./temp)*(k_s*f_soh/(k_p+k_s*f_pch2oh+k_s*f_soh)); {&1759, 3031} // Branching ratios estimated with SAR for H-
abstraction rate constants by OH.
<G43070b> NPROPOL + OH       = HYPROPO2 + H2O                        : {%TrG} 4.6E-12*EXP(70./temp)*((k_p+k_s*f_pch2oh)/(k_p+k_s*f_pch2oh+k_s*f_soh)); {&1759, 3031} // Branching ratios estimated with SAR
for H-abstraction rate constants by OH.
<G43071a> PROPENOL + OH      = HCOOH + OH + CH3CHO                   : {%TrG} k_CH2CHOH_OH_HCOOH; {&3031, 3179} // \onlythischannel
<G43072>  PROPENOL + HCOOH   = C2H5CHO + HCOOH                       : {%TrG} k_CH2CHOH_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G43073>  C2H5CHO  + HCOOH   = PROPENOL + HCOOH                      : {%TrG} k_ALD_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G43074>  HCOCOCH2OOH + OH   = HCOCO + CO + HO2 + OH                 : {%TrG} k_s*f_sooh*f_co+.6*k_CH3OOH_OH; {&3031} // HCOCOCHO would be produced but undergoes fast photolysis (faster than MGLYOX) and is
substituted with its products.
<G43202>  HCOCH2CHO + OH     = HCOCH2CO3                           : {%TrGTer} 4.29E-11; {&2419}
<G43203>  HCOCH2CHO + NO3    = HCOCH2CO3 + HNO3                    : {%TrGTer} 2.*KNO3AL*2.4; {&2419}
<G43204a> HCOCH2CO3          = HCOCH2O2 + CO2                      : {%TrGTer} k1_RO2RC03*0.9; {&3031}
<G43204b> HCOCH2CO3          = HCOCH2CO2H                          : {%TrGTer} k1_RO2RC03*0.1; {&3031}
<G43205>  HCOCH2CO3 + NO     = HCOCH2O2 + CO2 + NO2                : {%TrGTer} KAPNO; {&2419}
<G43206>  HCOCH2CO3 + NO2    = C3PAN2                              : {%TrGTer} k_CH3CO3_NO2; {&2419}
<G43207a> HCOCH2CO3 + HO2    = HCOCH2CO3H                          : {%TrGTer} KAPHO2*rco3_ooh; {&2419}
<G43207b> HCOCH2CO3 + HO2    = HCOCH2CO2H + O3                     : {%TrGTer} KAPHO2*rco3_o3; {&2419}
<G43207c> HCOCH2CO3 + HO2    = HCOCH2O2 + CO2 + OH                 : {%TrGTer} KAPHO2*rco3_oh; {&2419}
<G43210>  C3PAN2             = HCOCH2CO3 + NO2                     : {%TrGTer} k_PAN_M; {&2419}
<G43211>  C3PAN2 + OH        = GLYOX + CO + NO2                    : {%TrGTer} 2.10E-11; {&2419}
<G43212>  HCOCH2CO2H + OH    = HCOCH2O2 + CO2                      : {%TrGTer} 2.14E-11; {&2419}
<G43213a> HOC2H4CO3          = HOCH2CH2O2 + CO2                    : {%TrGTer} k1_RO2RC03*0.9; {&3031}
<G43213b> HOC2H4CO3          = HOC2H4CO2H                          : {%TrGTer} k1_RO2RC03*0.1; {&3031}
<G43214>  HOC2H4CO3 + NO     = HOCH2CH2O2 + CO2 + NO2              : {%TrGTer} KAPNO; {&2419}
<G43215a> HOC2H4CO3 + HO2    = HOC2H4CO3H                          : {%TrGTer} KAPHO2*rco3_ooh; {&2419}
<G43215b> HOC2H4CO3 + HO2    = HOCH2CH2O2 + CO2 + OH               : {%TrGTer} KAPHO2*rco3_oh; {&2419}
<G43215c> HOC2H4CO3 + HO2    = HOC2H4CO2H + O3                     : {%TrGTer} KAPHO2*rco3_o3; {&2419}
<G43218>  HOC2H4CO3 + NO2    = C3PAN1                              : {%TrGTer} k_CH3CO3_NO2; {&2419}
<G43219>  HOC2H4CO2H + OH    = HOCH2CH2O2 + CO2                    : {%TrGTer} 1.39E-11; {&2419}
<G43220>  HOC2H4CO3H + OH    = HOC2H4CO3                           : {%TrGTer} 1.73E-11; {&2419}
<G43221>  C3PAN1             = HOC2H4CO3 + NO2                     : {%TrGTer} k_PAN_M; {&2419}
<G43222>  C3PAN1 + OH        = HOCH2CHO + CO + NO2                 : {%TrGTer} 4.51E-12; {&2419}
<G43223>  HCOCH2CO3H + OH    = HCOCH2O2 + CO2 + H2O                : {%TrGTer} 2.49E-11; {&2419} // Products simplified
<G43415>  C3DIALOOH  + OH    = C33CO + OH                  : {%TrGAro} 1.44E-10; {&2419}
<G43418a> C3DIALO2   + HO2   = C3DIALOOH                   : {%TrGAro} KRO2HO2(3)*(rco3_ooh+rco3_o3); {&2419}
<G43418b> C3DIALO2   + HO2   = GLYOX + CO + HO2 + OH       : {%TrGAro} KRO2HO2(3)*rco3_oh; {&2419}
<G43419>  C3DIALO2   + NO    = GLYOX + CO + HO2 + NO2      : {%TrGAro} KRO2NO; {&2419} // KDEC C3DIALO $\rightarrow$ GLYOX + CO + HO2
<G43420>  C3DIALO2   + NO3   = GLYOX + CO + HO2 + NO2      : {%TrGAro} KRO2NO3; {&2419} // KDEC C3DIALO $\rightarrow$ GLYOX + CO + HO2
<G43421>  C3DIALO2           = GLYOX + CO + HO2            : {%TrGAro} k1_RO2s0RO2; {&2419} // Permutation reaction (minor channels removed).
<G43422a> HCOCOHCO3  + HO2   = GLYOX + CO2 + HO2 + OH      : {%TrGAro} KAPHO2*rco3_oh; {&2419}
<G43422b> HCOCOHCO3  + HO2   = HCOCOHCO3H                  : {%TrGAro} KAPHO2*(rco3_ooh+rco3_o3); {&2419}
<G43424>  HCOCOHCO3  + NO    = GLYOX + CO2 + HO2 + NO2     : {%TrGAro} KAPNO; {&2419}
<G43425>  HCOCOHCO3  + NO2   = HCOCOHPAN                   : {%TrGAro} k_CH3CO3_NO2; {&2419}
<G43426>  HCOCOHCO3  + NO3   = GLYOX + CO2 + HO2 + NO2     : {%TrGAro} KRO2NO3*1.74; {&2419}
<G43427>  HCOCOHCO3          = GLYOX + CO2 + HO2           : {%TrGAro} k1_RO2RC03; {&2419}
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<G43428>  METACETHO  + OH   = CH3CO + CO2               : {%TrGAro} 9.82E-11; {&2419}
<G43442>  HOCOCHPAN  + OH   = GLYOX + CO + NO2          : {%TrGAro} 6.97E-11; {&2419}
<G43443>  HOCOCHPAN         = HOCOCHCO3 + NO2           : {%TrGAro} k_PAN_M; {&2419}
<G43444>  C320H13CO  + OH   = HOCOCHCO3                 : {%TrGAro} 1.36E-10; {&2419}
<G43446>  HOCOCHCO3H + OH   = HOCOCHCO3                 : {%TrGAro} 7.33E-11; {&2419}
<G44000>  NC4H10     + OH   = LC4H9O2 + H2O                                   : {%TrG} 2.03E-17*temp*temp*EXP(78./temp); {&1759} // The \kpp{LC4H9O2} composition (\chem{nC_4H_9O_2}:\chem{sC_4H_9O_2}
ratio) is assumed to be equal to the ratio of the production rates at 298K: k\_p/(k\_p+k\_s) = 0.1273 and k\_s/(k\_p+k\_s) = 0.8727.
<G44001a> LC4H9O2           = C3H7CHO + HO2                                  : {%TrG} (k1_RO2pRO2*0.1273+k1_RO2sRO2*0.8727)*0.1273; {&2419, 3031}
<G44001b> LC4H9O2           = .636 MEK + .636 HO2 + .364 CH3CHO + .364 C2H5O2        : {%TrG} (k1_RO2pRO2*0.1273+k1_RO2sRO2*0.8727)*0.8727; {&2419, 3031} // \chem{sC_4H_9O_2} products are substituted with
0.636 \kpp{MEK} + \kpp{HO2} and 0.364 \kpp{CH3CHO} + \kpp{C2H5O2} at 1 bar and 298 K.
<G44002>  LC4H9O2     + HO2 = LC4H9OOH                                       : {%TrG} KRO2HO2(4); {&2419}
<G44003a> LC4H9O2     + NO  = NO2 + C3H7CHO + HO2                            : {%TrG} KRO2NO*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.1273; {&2419, 3031}
<G44003b> LC4H9O2     + NO  = NO2 + .636 MEK + .636 HO2 + .364 CH3CHO + .364 C2H5O2 : {%TrG} KRO2NO*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.8727; {&2419, 3031}
<G44003c> LC4H9O2     + NO  = LC4H9NO3                                       : {%TrG} KRO2NO*(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)); {&2419} // The alkyl nitrate
yield is the weighted average yield for the two isomers forming from \chem{nC_4H_9O_2} and \chem{sC_4H_9O_2}.
<G44004a> LC4H9O2     + NO3 = NO2 + C3H7CHO + HO2                            : {%TrG} KRO2NO3*0.1273; {&2419, 3031}
<G44004b> LC4H9O2     + NO3 = NO2 + .636 MEK + .636 HO2 + .364 CH3CHO + .364 C2H5O2 : {%TrG} KRO2NO3*0.8727; {&2419, 3031}
<G44005a> LC4H9OOH    + OH  = LC4H9O2 + H2O                          : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44005b> LC4H9OOH    + OH  = C3H7CHO + H2O + OH                     : {%TrG} k_s*f_tooh*f_alk*(k_p/(k_p+k_s)); {&3031}
<G44005c> LC4H9OOH    + OH  = MEK + H2O + OH                         : {%TrG} k_t*f_tooh*f_alk*(k_s/(k_p+k_s)); {&3031}
<G44006a> IC4H10      + OH  = TC4H9O2 + H2O                          : {%TrG} 1.17E-17*temp*temp*EXP(213./temp)*k_t/(3.*k_p+k_t); {&1627}
<G44006b> IC4H10      + OH  = IC4H9O2 + H2O                          : {%TrG} 1.17E-17*temp*temp*EXP(213./temp)*3.*k_p/(3.*k_p+k_t); {&1627}
<G44007>  TC4H9O2           = CH3COCH3 + CH3                         : {%TrG} k1_RO2tRO2; {&2419, 3031}
<G44008>  TC4H9O2     + HO2 = TC4H9OOH                               : {%TrG} KRO2HO2(4); {&2419}
<G44009a> TC4H9O2     + NO  = NO2 + CH3COCH3 + CH3                   : {%TrG} KRO2NO*(1.-alpha_AN(4,3,0,0,0,temp,cair)); {&2419, 3031}
<G44009b> TC4H9O2     + NO  = TC4H9NO3                               : {%TrG} KRO2NO*alpha_AN(4,3,0,0,0,temp,cair); {&2419}
<G44010a> TC4H9OOH    + OH  = TC4H9O2 + H2O                          : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44010b> TC4H9OOH    + OH  = CH3COCH3 + HCHO + OH + H2O             : {%TrG} 3.*k_p*f_tch2oh; {&3031} // H-abstraction from primary C and substitution of the resulting peroxy radical with its products from
the reaction with NO.
<G44011>  TC4H9NO3    + OH  = CH3COCH3 + HCHO + NO2 + H2O            : {%TrG} 3.*k_p*f_ch2ono2; {&3031} // H-abstraction from primary C and substitution of the resulting peroxy radical with its products from
the reaction with NO.
<G44012>  IC4H9O2           = IPRCHO                                 : {%TrG} k1_RO2sRO2; {&2419, 3031}
<G44013>  IC4H9O2     + HO2 = IC4H9OOH                               : {%TrG} KRO2HO2(4); {&2419}
<G44014a> IC4H9O2     + NO  = NO2 + IPRCHO                           : {%TrG} KRO2NO*(1.-alpha_AN(4,2,0,0,0,temp,cair)); {&2419, 3031}
<G44014b> IC4H9O2     + NO  = IC4H9NO3                               : {%TrG} KRO2NO*alpha_AN(4,2,0,0,0,temp,cair); {&2419}
<G44015a> IC4H9OOH    + OH  = IC4H9O2 + H2O                          : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44015b> IC4H9OOH    + OH  = IPRCHO + OH + H2O                      : {%TrG} k_s*f_sooh+2.*k_s+k_t*f_pch2oh; {&3031} // Products assumed to be only from H-abstraction from a secondary C bearing the -OOH
group.
<G44016>  IC4H9NO3    + OH  = IPRCHO + NO2 + H2O                     : {%TrG} k_s*f_ono2+2.*k_p+k_t*f_ch2ono2; {&3031} // Products assumed to be only from H-abstraction from a secondary C bearing the -
\chem{ONO_2} group.
<G44017>  MVK         + O3  = .87 MGLYOX + .5481 CO + .1392 HO2 + .1392 OH + .3219 CH2OO + .13 HCHO + .0468O OH + .0468O CO + .07280 CH3CO + .026 CH3CHO + .026 CO2 + .026 HCHO + .026 HO2 + .02402  MGLYOX +
.02402 H2O2 + .00718 CH3COCO2H    : {%TrG} 8.5E-16*EXP(-1520./temp); {&3031}
<G44018>  MVK         + OH  = LHMVKABO2                              : {%TrG} 2.6E-12*EXP(610./temp); {&3031, 1759} // LHMVKABO2 is 0.12 HMVKAO2 + 0.88 HMVKBO2.
<G44019>  MEK         + OH  = LMEKO2 + H2O                           : {%TrG} 1.5E-12*EXP(-90./temp); {&1759, 3031} // \kpp{LMEKO2} represents 0.62 MEKBO2 + 0.38 MEKAO2.
<G44020>  LMEKO2      + HO2 = LMEKOOH                                : {%TrG} KRO2HO2(4); {&3031}
<G44021a> LMEKO2 {+O2}+ NO  = .62 CH3CHO + .62 CH3CO + .38 HCHO + .38 CO2 + .38 HOCH2CH2O2 + NO2 : {%TrG} KRO2NO*(1.-(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair))); {&3031} // The
products of MEKAO are substituted with \kpp{HCHO} + \kpp{CO2} + \kpp{HOCH2CH2O2}.
<G44021b> LMEKO2 {+O2}+ NO  = LMEKNO3                              : {%TrG} KRO2NO*(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair)); {&3031}
<G44022a> LMEKOOH     + OH  = LMEKO2 + H2O                           : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44022b> LMEKOOH     + OH  = .62 BIACET + .38 HCHO + .38 CO2 + .38 HOCH2CH2O2 + H2O + OH            : {%TrG} (.62*k_t*f_tooh*f_co+.38*k_s*f_sooh); {&3031}
<G44023a> LC4H9NO3    + OH  = MEK + NO2 + H2O                        : {%TrG} (k_t*f_ono2*f_alk+k_p*f_alk+k_s*f_ch2ono2+k_p)*(k_s/(k_p+k_s)); {&3031} // Products from H-abstraction from the tertiary carbon
bearing the \chem{ONO_2} group.
<G44023b> LC4H9NO3    + OH  = C3H7CHO + NO2 + H2O                    : {%TrG} (k_p+k_s*(1+f_ch2ono2+f_ono2)*f_alk)*(k_p/(k_p+k_s)); {&3031} // Products from H-abstraction from the secondary carbon bearing the
\chem{ONO_2} group.
<G44024>  MPAN        + OH  = ACETOL + CO + NO2                      : {%TrG} 3.2E-11; {&1629}
<G44025>  MPAN {+M}         = MACO3 + NO2                            : {%TrG} k_PAN_M; // Same value as for \kpp{PAN}.
<G44026>  LMEKO2            = .538 HCHO + .538 CO2 + .459 HOCH2CH2O2 + .079 C2H5O2 + .462 CH3CO + .462 CH3CHO : {%TrG} (.62*k1_RO2s0RO2+.38*k1_RO2p0RO2); {&2419} // Products as in G4415. Only the main
channels for each isomer are considered. Weighted average for the isomers.
<G44027>  MACR        + OH  = .45 MACO3 + .55 MACRO2                 : {%TrG} 8.E-12*EXP(380./temp); {&3147, 3031}
<G44028>  MACR        + O3  = .5481 CO +  .1392 HO2 + .1392 OH + .3219 CH2OO + .87 MGLYOX + .13 HCHO +  .13 OH + .065 CHOCOCH2O2 + .065 CO + .065 CH3CO    : {%TrG} 1.36E-15*EXP(-2112./temp); {&3031}
<G44029>  MACR        + NO3 = MACO3 + HNO3                           : {%TrG} KNO3AL*2.0; {&2419}
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<G44030a> MACO3             = CH3CO + HCHO + CO2                    : {%TrG} kl_RO2RCO3*0.9; {&3031}
<G44030b> MACO3             = MACO2H                                : {%TrG} kl_RO2RCO3*0.1; {&3031}
<G44031a> MACO3       + HO2 = MACO2 + OH                            : {%TrG} KAPHO2*rco3_oh; {&3031}
<G44031b> MACO3       + HO2 = MACO3H                                : {%TrG} KAPHO2*rco3_ooh; {&3031}
<G44031c> MACO3       + HO2 = MACO2H + O3                           : {%TrG} KAPHO2*rco3_o3; {&3031}
<G44032>  MACO3       + NO  = MACO2 + NO2                           : {%TrG} 8.7DE-12*EXP(290./temp); {&3031}
<G44033>  MACO3       + NO2 = MPAN                                  : {%TrG} k_CH3CO3_NO2; {&2419}
<G44034>  MACO3       + NO3 = MACO2 + NO2                           : {%TrG} KRO2NO3*1.6D; {&3031}
<G44035>  MACR02            = .7 ACETOL + .7 HCHO + .7 HO2 + .3 MACROH : {%TrG} kl_RO2toRO2; {&2419} // Rate constant replaced with the one of beta hydroxy \chem{RO_2}.
<G44036a> MACR02      + HO2 = MACRO + OH                            : {%TrG} KRO2HO2(4)*rcoch2o2_oh; {&3031}
<G44036b> MACR02      + HO2 = MACROOH                               : {%TrG} KRO2HO2(4)*rcoch2o2_ooh; {&3031}
<G44037a> MACR02      + NO  = MACRO + NO2                           : {%TrG} KRO2NO*(1.-alpha_AN(6,3,1,0,0,temp,cair)); {&3031}
<G44037b> MACR02      + NO  = MACRN                                 : {%TrG} KRO2NO*alpha_AN(6,3,1,0,0,temp,cair); {&3031}
<G44038>  MACR02      + NO3 = MACRO + NO2                           : {%TrG} KRO2NO3; {&3031}
<G44039a> MACROOH     + OH  = MACRO2                                : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44039b> MACROOH     + OH  = CO + ACETOL + OH                      : {%TrG} k_t*f_o*f_tch2oh*f_alk; {&3031}
<G44039c> MACROOH     + OH  = CO + MGLYOX + HO2                     : {%TrG} (k_s*f_soh*f_pch2oh + k_rohro); {&3031}
<G44040>  MACROH      + OH  = ACETOL + CO + HO2                     : {%TrG} k_t*f_o*f_tch2oh*f_alk; {&3031}
<G44041>  MACRO             = .885 ACETOL + .885 CO + .115 MGLYOX + .115 HCHO + HO2  : {%TrG} KDEC; {&3031}
<G44042>  MACO2H      + OH  = ACETOL + HO2 + CO2                    : {%TrG} ((k_adt+k_adp)*a_co2h+k_co2h); {&3031}
<G44043a> MACO3H      + OH  = ACETOL + CO2 + OH                     : {%TrG} (k_adt+k_adp)*a_co2h; {&3031}
<G44043b> MACO3H      + OH  = MACO3                                 : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44044>  LHMVKAB02         = .024 CO2H3CHO + .072 MGLYOX + .072 HO2 + .072 HCHO + .528D CH3CO + .528D HOCH2CHO + .176 BIACETOH + .2 HO12CO3C4 : {%TrG} (.12*kl_RO2pORO2+.88*kl_RO2sORO2); {&3031}
<G44045a> LHMVKAB02   + HO2 = OH + HOCH2CHO + CH3CO                 : {%TrG} KRO2HO2(4)*.88*rcoch2o2_oh; {&3031}
<G44045b> LHMVKAB02   + HO2 = LHMVKAB0OH                            : {%TrG} KRO2HO2(4)*(.12+.88*rcoch2o2_ooh); {&3031}
<G44046a> LHMVKAB02   + NO  = .12 MGLYOX + .12 HO2 + .88 HOCH2CHO + .88 CH3CO + .12 HCHO + NO2 : {%TrG} KRO2NO*(1.-(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair))); {&3031}
<G44046b> LHMVKAB02   + NO  = MVKNO3                                : {%TrG} KRO2NO*(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair)); {&3031} // Using value for secondary nitrate (88\%
of total).
<G44047>  LHMVKAB02   + NO3 = .12 MGLYOX + .12 HO2 + .88 HOCH2CHO + .88 CH3CO + .12 HCHO + .12 HO2 + NO2 : {%TrG} KRO2NO3; {&3031}
<G44048a> LHMVKAB0OH  + OH  = LHMVKAB02                             : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44048b> LHMVKAB0OH  + OH  = .12 CO2H3CHO + .88 BIACETOH + OH      : {%TrG} (.12*k_s*f_sooh*f_pch2oh+.88*k_t*f_tooh*f_pch2oh*f_co); {&3031}
<G44049a> CO2H3CHO    + OH  = CO2H3CO3                              : {%TrG} k_t*f_o*f_alk; {&3031}
<G44049b> CO2H3CHO    + OH  = CO23C3CHO + HO2 + H2O                 : {%TrG} k_t*f_co*f_toh*f_cho; {&3031}
<G44050>  CO2H3CHO    + NO3 = CO2H3CO3 + HNO3                       : {%TrG} KNO3AL*4.0; {&2419}
<G44051>  CO2H3CO3          = MGLYOX + HO2 + CO2                    : {%TrG} kl_RO2RCO3; {&3031}
<G44052a> CO2H3CO3    + HO2 = OH + MGLYOX + HO2 + CO2               : {%TrG} KAPHO2*rco3_oh; {&3031}
<G44052b> CO2H3CO3    + HO2 = CO2H3CO2H + O3                        : {%TrG} KAPHO2*rco3_o3; {&3031}
<G44052c> CO2H3CO3    + HO2 = CO2H3CO3H                             : {%TrG} KAPHO2*rco3_ooh; {&3031}
<G44053>  CO2H3CO3    + NO  = MGLYOX + HO2 + NO2  + CO2             : {%TrG} KAPNO; {&3031}
<G44054>  CO2H3CO3    + NO3 = MGLYOX + HO2 + NO2  + CO2             : {%TrG} KRO2NO3*1.6D; {&3031}
<G44055a> CO2H3CO3H   + OH  = CO2H3CO3                              : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G44055b> CO2H3CO3H   + OH  = CH3CO + CO + CO2 + OH                 : {%TrG} (k_t*f_co2h*f_co*f_toh); {&3031}
<G44055b> CO2H3CO2H   + OH  = CH3CO3CO2H + HO2                      : {%TrG} k_t*f_co2h*f_co*f_toh+k_co2h; {&3031}
<G44057a> HO12CO3C4   + OH  = BIACETOH + HO2                        : {%TrG} k_t*f_toh*f_alk*f_co; {&3031}
<G44057b> HO12CO3C4   + OH  = CO2H3CHO + HO2                        : {%TrG} k_s*f_soh*f_alk; {&3031}
<G44058>  MACO2             = .65 CH3 + .65 CO + .65 HCHO + .35 OH + .35 CH3CO3CH2O2 + CO2  : {%TrG} KDEC; {&3031}
<G44059>  LHMVKAB02         = .88 MGLYOX + .88 HCHO + .12 HOOCH2CHO + .12 CH3CO + OH   : {%TrG} KHSD; {&3031}
<G44060>  MACR02            = MGLYOX + HCHO + OH                    : {%TrG} KHSB; {&3031}
<G44061a> MVKNO3 + OH       = MGLYOX + CO2 + HO2 + NO2 + H2O        : {%TrG} k_s*f_sooh*f_ch2ono2+k_rohro; {&3031} // Using value for secondary nitrate (88\% of total).
<G44061b> MVKNO3 + OH       = BIACETOH + NO2 + H2O                  : {%TrG} k_t*f_ono2*f_co*f_pch2oh; {&3031} // Using value for secondary nitrate (88\% of total).
<G44062a> MACRN + OH        =  ACETOL + CO2 + NO2 + H2O             : {%TrG} k_t*f_o*f_ch2ono2; {&3031} // Simplified products.
<G44062b> MACRN + OH        =  MGLYOX + CO + NO2 + H2O              : {%TrG} k_rohro+k_s*f_sooh*f_ch2ono2; {&3031} // Simplified products.
<G44063>  MACR02            = ACETOL + OH + CO                      : {%TrG} Kl4HSAL; {&3031}
<G44064>  EZCH3CO2CHCHO     = .9 CH3COCHCO + .1 CH3CO + .01 GLYOX + .18 CO + .09 HO2 + OH     : {%TrG} K15HS24VYNAL; {&3031}
<G44065>  EZCH3CO2CHCHO + HO2=  CH3COOHCHCHO                        : {%TrG} KRO2HO2(4); {&3031}
<G44066>  EZCH3CO2CHCHO + NO =  CH3COCHO2CHO + NO2                  : {%TrG} KRO2NO; {&3031} // \alkylnitrateneglected
<G44067>  EZCH3CO2CHCHO + NO3=  CH3COCHO2CHO + NO2                  : {%TrG} kRO2NO3; {&3031}
<G44068>  EZCH3CO2CHCHO      =  CH3COCHO2CHO                        : {%TrG} kl_RO2sORO2; {&3031}
<G44069>  EZCHOCCH3CHO2      =  HCOCCH3CO + OH                      : {%TrG} K15HS24VYNAL; {&3031}
<G44070>  EZCHOCCH3CHO2 + NO =  HCOCO2CH3CHO + NO2                  : {%TrG} KRO2NO; {&3031} // \alkylnitrateneglected
<G44071>  EZCHOCCH3CHO2 + HO2=  HCOCCH3CHOOH                        : {%TrG} KRO2HO2(4); {&3031}
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<G44072>  EZCH0CCH3CH02 + N03=  HC0C02CH3CH0 + N02               : {%TrG} KR02N03; {&3031}
<G44073>  EZCH0CCH3CH02      =  HC0C02CH3CH0                    : {%TrG} k1_R02p0R02; {&3031}
<G44074>  CH3C00HCHCH0       =  CH3C0CH02CH0 + 0H               : {%TrG} KHYDEC; {&3031}
<G44075>  HC0CCH3CH00H       =  HC0C02CH3CH0 + 0H               : {%TrG} KHYDEC; {&3031}
<G44076>  CH3C0CH02CH0 + N0  =  CH3C0 + GLY0X + N02             : {%TrG} KR02N0; {&3031} // \alkylnitrateneglected
<G44077>  CH3C0CH02CH0 + N03 =  CH3C0 + GLY0X + N02             : {%TrG} KR02N03; {&3031}
<G44078>  CH3C0CH02CH0 + H02 =  CH3C0 + GLY0X + 0H              : {%TrG} KR02H02(4); {&3031} // 0ther channel neglected.
<G44079>  CH3C0CH02CH0       =  CH3C0 + GLY0X                   : {%TrG} k1_R02s0R02; {&3031}
<G44080>  HC0C02CH3CH0       =  MGLY0X + C0 + H02               : {%TrG} k1_R02t0R02; {&3031}
<G44081>  HC0C02CH3CH0 + N0  =  MGLY0X + C0 + H02 + N02         : {%TrG} KR02N0; {&3031} // \alkylnitrateneglected
<G44082>  HC0C02CH3CH0 + H02 =  MGLY0X + C0 + H02 + 0H          : {%TrG} KR02H02(4); {&3031} // 0ther channel neglected.
<G44083>  HC0C02CH3CH0 + N03 =  MGLY0X + C0 + H02 + N02         : {%TrG} KR02N03; {&3031}
<G44084>  HC0CCH3C0  + 0H    =  C0 + MGLY0X + H02               : {%TrG} 1E-10*a_cho; {&3155, 3031}
<G44085>  CH3C0CHC0  + 0H    = C0 + MGLY0X + H02                : {%TrG} 7.6E-11*a_coch3; {&3155, 3031} // k for \chem{CH_3CHC0} from \cite{3155} adjusted.
<G44086>  LMEKN03  + 0H      = .62 MGLY0X + .62 HCH0 + .62 H02 + .62 N02 + .38 CH3C0 + .38 N03CH2CH0 : {%TrG} .62*(k_p*(f_co+f_ch2ono2))+.38*(k_s*f_ch2ono2*f_co); {&3031} // Simplified product distribution.
<G44087>  MEPR0PENE + 0H    = IBUT0LB02                        : {%TrG} 9.4E-12*EXP(505./temp); {&1759}
<G44088a> MEPR0PENE + 03    = CH3C0CH3 + CH200A                : {%TrG} 2.7E-15*EXP(-1630./temp)*0.33; {&1759, 3031}
<G44088b> MEPR0PENE + 03    = CH3C0CH202 + 0H + HCH0           : {%TrG} 2.7E-15*EXP(-1630./temp)*0.67; {&1759, 3031}
<G44089>  MEPR0PENE + N03   = CH3C0CH3 + HCH0 + N02            : {%TrG} 3.4E-13; {&1759, 3031} // The nitrated \chem{R0_2} is replaced by its products upon reaction with N0.
<G44090>  IBUT0LB02         = CH3C0CH3 + HCH0 + H02            : {%TrG} k1_R02t0R02; {&3031}
<G44091a> IBUT0LB02 + H02   = IBUT0LB00H                       : {%TrG} KR02H02(4)*rcoch2o2_ooh; {&3031}
<G44091b> IBUT0LB02 + H02   = CH3C0CH3 + HCH0 + H02 + 0H       : {%TrG} KR02H02(4)*rcoch2o2_oh; {&3031}
<G44092a> IBUT0LB02 + N0    = CH3C0CH3 + HCH0 + H02 + N02      : {%TrG} KR02N0*(1.-alpha_AN(5,3,0,0,0,temp,cair)); {&3031}
<G44092b> IBUT0LB02 + N0    = IBUT0LBN03                       : {%TrG} KR02N0*alpha_AN(5,3,0,0,0,temp,cair); {&3031}
<G44093>  IBUT0LB02 + N03   = CH3C0CH3 + HCH0 + H02 + N02      : {%TrG} KR02N03; {&3031}
<G44094a> IBUT0LB00H + 0H   = IBUT0LB02                        : {%TrG} .6*k_CH300H_0H; {&3031}
<G44094b> IBUT0LB00H + 0H   = CH3C0CH3 + HCH0 + H02            : {%TrG} k_s*f_sooh*f_pch2oh; {&3031}
<G44095>  IBUT0LBN03 + 0H   = CH3C0CH3 + HCH0 + H02 + N02      : {%TrG} 3.*k_p; {&3031}
<G44096>  BUT1ENE    + 0H   = LBUT1EN02                        : {%TrG} 6.6E-12*EXP(465./temp); {&1759} // Both LBUT1EN02 isomers mostly \chem{C_2H_5CH0}.
<G44097a> BUT1ENE + 03      = HCH0 + .5 C2H5CH0 + .5 H202 + .5 CH3CH0 + .5 C0 + .5 H02 : {%TrG} 3.35E-15*EXP(-1745./temp)*.57; {&1759, 3031} // Branching ratios according to \citet{3200}.
\chem{CH_3CH0_2CH0} is replaced with its major products \chem{CH_3CH0} + C0 + \chem{H0_2}.
<G44097b> BUT1ENE + 03      = C2H5CH0 + CH200A                 : {%TrG} 3.35E-15*EXP(-1745./temp)*.43; {&1759, 3031} // Branching ratios according to \citet{3200}.
<G44098>  BUT1ENE + N03     = C2H5CH0 + HCH0 + N02             : {%TrG} 3.2E-13*EXP(-950./temp); {&1759, 3031} // The nitrated \chem{R0_2} is replaced by its products upon reaction with N0.
<G44099>  LBUT1EN02         = C2H5CH0 + HCH0 + H02             : {%TrG} k1_R02s0R02; {&3031}
<G44100a> LBUT1EN02 + H02   = LBUT1EN00H                       : {%TrG} KR02H02(4)*rcoch2o2_ooh; {&3031}
<G44100b> LBUT1EN02 + H02   = C2H5CH0 + HCH0 + H02 + 0H        : {%TrG} KR02H02(4)*rcoch2o2_oh; {&3031}
<G44101a> LBUT1EN02 + N0    = C2H5CH0 + HCH0 + H02 + N02       : {%TrG} KR02N0*(1.-alpha_AN(5,2,0,0,0,temp,cair)); {&3031}
<G44101b> LBUT1EN02 + N0    = LBUT1ENN03                       : {%TrG} KR02N0*alpha_AN(5,2,0,0,0,temp,cair); {&3031}
<G44102>  LBUT1EN02 + N03   = C2H5CH0 + HCH0 + H02 + N02       : {%TrG} KR02N03; {&3031}
<G44103a> LBUT1EN00H  + 0H  = LBUT1EN02                        : {%TrG} .6*k_CH300H_0H; {&3031}
<G44103b> LBUT1EN00H  + 0H  = C2H5C03 + HCH0 + H02             : {%TrG} k_t*f_tooh*f_pch2oh; {&3031} // MEKC0H replaced by its major oxidation products.
<G44104>  LBUT1ENN03 + 0H   = C2H5CH0 + C0 + H02 + N02         : {%TrG} k_s*f_soh*f_ch2ono2; {&3031} // Carbonyl nitrate replaced by its major oxidation products.
<G44105>  CBUT2ENE + 0H     = BUT2OL02                         : {%TrG} 1.1E-11*EXP(485./temp); {&1759}
<G44106>  CBUT2ENE + 03     = CH3CH0 + .16 CH3CH0H00H + .50 0H + .50 HC0CH202 + .05 CH2C0 + .09 CH30H + .09 C0 + .2 CH4 + .2 C02: {%TrG} 3.2E-15*EXP(-965./temp); {&1759, 3031} // CH3CH00A products as from
\chem{C_3H_6} + \chem{0_3} reaction.
<G44107>  CBUT2ENE + N03    = 2 CH3CH0 + N02                   : {%TrG} 3.5E-13; {&1759, 3031} // The nitrated \chem{R0_2} is replaced by its products upon reaction with N0.
<G44108>  TBUT2ENE + 0H     = BUT2OL02                         : {%TrG} 1.0E-11*EXP(553./temp); {&1759}
<G44109>  TBUT2ENE + 03     = CH3CH0 + .16 CH3CH0H00H + .50 0H + .50 HC0CH202 + .05 CH2C0 + .09 CH30H + .09 C0 + .2 CH4 + .2 C02: {%TrG} 6.6E-15*EXP(-1060./temp); {&1759, 3031}
<G44110>  TBUT2ENE + N03    = 2 CH3CH0 + N02                   : {%TrG} 1.78E-12*EXP(-530./temp)+1.28E-14*EXP(570./temp); {&1759, 3031} // The nitrated \chem{R0_2} is replaced by its products upon reaction with
N0.
<G44111>  BUT2OL02          = C2H5CH0 + HCH0 + H02             : {%TrG} k1_R02s0R02; {&3031}
<G44112a> BUT2OL02 + H02    = BUT2OL00H                        : {%TrG} KR02H02(4)*rcoch2o2_ooh; {&3031}
<G44112b> BUT2OL02 + H02    = 2 CH3CH0 + H02 + 0H              : {%TrG} KR02H02(4)*rcoch2o2_oh; {&3031}
<G44113a> BUT2OL02 + N0     = 2 CH3CH0 + H02 + N02             : {%TrG} KR02N0*(1.-alpha_AN(5,2,0,0,0,temp,cair)); {&3031}
<G44113b> BUT2OL02 + N0     = BUT2OLN03                        : {%TrG} KR02N0*alpha_AN(5,2,0,0,0,temp,cair); {&3031}
<G44114>  BUT2OL02 + N03    = 2 CH3CH0 + H02 + N02             : {%TrG} KR02N03; {&3031}
<G44115a> BUT2OL00H  + 0H   = BUT2OL02                         : {%TrG} .6*k_CH300H_0H; {&3031}
<G44115b> BUT2OL00H  + 0H   = LMEK00H + H02                    : {%TrG} k_t*f_toh*f_pch2oh; {&3031}
<G44115c> BUT2OL00H  + 0H   = BUT2OL0 + 0H                     : {%TrG} k_t*f_tooh*f_pch2oh; {&3031}
<G44116>  BUT2OLN03  + 0H   = LMEKN03 + H02                    : {%TrG} k_t*f_toh*f_ch2ono2; {&3031}
<G44117>  BUT2OL0    + 0H   = BIACET + H02                     : {%TrG} k_t*f_toh*f_co; {&3031}
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<G44118>  IPRCHO + OH       = IPRCO3 + H2O              : {%TrG} 6.8E-12*EXP(410./temp); {&1759}
<G44119>  IPRCHO + NO3      = IPRCO3 + HNO3             : {%TrG} 1.67E-12*EXP(-1460./temp); {&1759}
<G44120>  IPRCO3            = IC3H7O2 + CO2             : {%TrG} k1_RO2RCO3; {&2419}
<G44121a> IPRCO3 + HO2      = PERIBUACID                : {%TrG} KAPHO2*rco3_ooh; {&2419, 3031}
<G44121b> IPRCO3 + HO2      = IC3H7O2 + CO2 + OH        : {%TrG} KAPHO2*(1-rco3_ooh); {&2419, 3031}
<G44122>  IPRCO3 + NO2      = PIPN                      : {%TrG} k_CH3CO3_NO2; {&2419}
<G44123>  IPRCO3 + NO       = IC3H7O2 + CO2 + NO2       : {%TrG} KAPNO; {&2419}
<G44124a> PERIBUACID + OH   = IPRCO3 + H2O              : {%TrG} .6*k_CH3OOH_OH; {&2419}
<G44124b> PERIBUACID + OH   = CH3COCH3 + H2O + CO2      : {%TrG} k_s*f_co2h; {&3031} // Skipping intermediate steps mostly leading to acetone.
<G44125>  PIPN      {+ M}   = IPRCO3 + NO2              : {%TrG} k_PAN_M; {&2419}
<G44126>  PIPN + OH         = CH3COCH3 + CO2 + NO2      : {%TrG} k_s*f_cpan; {&3031} // Skipping intermediate steps mostly leading to acetone.
<G44127>  MPROPENOL + OH    = HCOOH + OH + CH3COCH3     : {%TrG} k_CH2CHOH_OH_HCOOH; {&3031, 3179} // \onlythischannel
<G44128>  MPROPENOL + HCOOH = IPRCHO + HCOOH            : {%TrG} k_CH2CHOH_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44129>  IPRCHO    + HCOOH = MPROPENOL + HCOOH         : {%TrG} k_ALD_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44130>  BUTENOL + OH      = HCOOH + OH + C2H5CHO      : {%TrG} k_CH2CHOH_OH_HCOOH; {&3031, 3179} // \onlythischannel
<G44131>  BUTENOL + HCOOH   = C3H7CHO + HCOOH           : {%TrG} k_CH2CHOH_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44132>  C3H7CHO + HCOOH   = BUTENOL + HCOOH           : {%TrG} k_ALD_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44133>  HVMK + OH         = HCOOH + OH + MGLYOX       : {%TrG} 8.8E-11; {&3031, 3179, 3185} // \onlythischannel
<G44134>  HVMK + HCOOH      =  CO2C3CHO + HCOOH         : {%TrG} k_CH2CHOH_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44135>  CO2C3CHO + HCOOH  = HVMK + HCOOH              : {%TrG} k_ALD_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44136>  HMAC + OH         = HCOOH + OH + MGLYOX       : {%TrG} 8.8E-11; {&3031, 3179, 3185} // \onlythischannel
<G44137>  HMAC + HCOOH      =  IBUTDIAL + HCOOH         : {%TrG} k_CH2CHOH_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44138>  IBUTDIAL  + HCOOH = HMAC + HCOOH              : {%TrG} k_ALD_HCOOH; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G44139>  CO2C3CHO  + OH    = CH3COCH2O2 + CO2 + H2O    : {%TrG} k_t*f_o*f_alk+k_s*f_cho*f_co; {&3031} // Simplified oxidation.
<G44140>  CO2C3CHO  + NO3   = CH3COCH2O2 + CO2 + HNO3   : {%TrG} KNO3AL*4.0; {&3031} // Simplified oxidation.
<G44141>  IBUTDIAL  + OH    = CH3CHO + CO + HO2 + CO2 + H2O  : {%TrG} 2.*k_t*f_o*f_alk+k_t*f_cho*f_cho; {&3031} // Simplified oxidation.
<G44142>  IBUTDIAL  + NO3   = CH3CHO + CO + HO2 + CO2 + HNO3 : {%TrG} 2.*KNO3AL*4.0; {&3031} // Simplified oxidation.
<G44200>  BIACET02           = CH3CO + HCHO + CO          : {%TrGTer} k1_RO2pORO2; {&2419}
<G44201>  BIACET02  + HO2    = BIACETOOH                  : {%TrGTer} KRO2HO2(4); {&2419}
<G44202>  BIACET02  + NO     = CH3CO + HCHO + CO + NO2    : {%TrGTer} KRO2NO; {&2419} // \alkylnitrateneglected
<G44203a> BIACETOOH + OH     = CO2C3CHO + OH              : {%TrGTer} k_s*f_co*f_sooh; {&2419} // Rate coefficient estimated with SAR \citep{3030}.
<G44203b> BIACETOOH + OH     = BIACET02                   : {%TrGTer} .6*k_CH3OOH_OH; {&2419}
<G44204>  C4402 + HO2        = C4400H                     : {%TrGTer} KRO2HO2(4); {&2419}
<G44205>  C4402 + NO         = HCOCH2CHO + CO2 + HO2 + NO2 : {%TrGTer} KRO2NO; {&2419} // \alkylnitrateneglected
<G44206>  C4402              = HCOCH2CHO + CO2 + HO2      : {%TrGTer} k1_RO2sORO2; {&2419}
<G44207>  C4400H + OH        = C4402                      : {%TrGTer} 7.4E-11; {&2419}
<G44208>  CHOC3CO2           = HCOCH2CO3 + HCHO           : {%TrGTer} k1_RO2pORO2; {&2419}
<G44209>  CHOC3CO2 + HO2     = C413COOH                   : {%TrGTer} KRO2HO2(4); {&2419}
<G44210>  CHOC3CO2 + NO      = HCOCH2CO3 + HCHO + NO2     : {%TrGTer} KRO2NO; {&2419} // \alkylnitrateneglected
<G44211>  C413COOH + OH      = CHOC3CO2                   : {%TrGTer} 8.33E-11; {&2419}
<G44212>  C4CODIAL + OH      = C312COCO3                  : {%TrGTer} 3.39E-11; {&2419}
<G44213>  C4CODIAL + NO3     = C312COCO3 + HNO3           : {%TrGTer} 2.*KNO3AL*4.0; {&2419}
<G44214>  C312COCO3          = CHOCOCH2O2 + CO2           : {%TrGTer} k1_RO2RCO3; {&2419}
<G44215a> C312COCO3 + HO2    = C312COCO3H                 : {%TrGTer} KAPHO2*rco3_ooh; {&2419}
<G44215b> C312COCO3 + HO2    = CHOCOCH2O2 + CO2 + OH      : {%TrGTer} KAPHO2*(1-rco3_ooh); {&2419}
<G44216>  C312COCO3 + NO2    = C312COPAN                  : {%TrGTer} k_CH3CO3_NO2; {&2419}
<G44217>  C312COCO3 + NO     = CHOCOCH2O2 + CO2 + NO2     : {%TrGTer} KAPNO; {&2419}
<G44218>  C312COCO3H + OH    = C312COCO3                  : {%TrGTer} 1.63E-11; {&2419}
<G44219>  C312COPAN          = C312COCO3 + NO2            : {%TrGTer} k_PAN_M; {&2419}
<G44220>  C312COPAN + OH     = C33CO + CO + NO2           : {%TrGTer} 1.27E-11; {&2419}
<G44221>  CO23C3CHO + OH     = CH3CO + 2 CO               : {%TrGTer} 8.4E-13*EXP(830./temp); {&3031} // Same k as for \kpp{MGLYOX} + \kpp{OH} \citep{1616}.
<G44222>  CO23C3CHO + NO3    = CH3CO + 2 CO + HNO3        : {%TrGTer} KNO3AL*4.0; {&2419}
<G44223>  IBUTALOH + OH      = IPRHOCO3                   : {%TrGTer} 1.4E-11; {&2419}
<G44224a> IPRHOCO3 + HO2     = CH3COCH3 + CO2 + HO2 + OH  : {%TrGTer} KAPHO2*rco3_oh; {&2419, 3031}
<G44224b> IPRHOCO3 + HO2     = IPRHOCO2H + O3             : {%TrGTer} KAPHO2*rco3_o3; {&2419, 3031}
<G44224c> IPRHOCO3 + HO2     = IPRHOCO3H                  : {%TrGTer} KAPHO2*rco3_ooh; {&2419, 3031}
<G44225>  IPRHOCO3 + NO      = CH3COCH3 + CO2 + HO2 + NO2 : {%TrGTer} KAPNO; {&2419}
<G44226>  IPRHOCO3 + NO2     = C4PAN5                     : {%TrGTer} k_CH3CO3_NO2; {&2419}
<G44227>  IPRHOCO3 + NO3     = CH3COCH3 + CO2 + HO2 + NO2 : {%TrGTer} KRO2NO3*1.74; {&2419}
<G44228a> IPRHOCO3           = CH3COCH3 + CO2 + HO2       : {%TrGTer} k1_RO2RCO3*0.7; {&2419}
<G44228b> IPRHOCO3           = IPRHOCO2H                  : {%TrGTer} k1_RO2RCO3*0.3; {&2419}
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<G44229>  IPRHOC02H + OH     = CH3COCH3 + CO2 + HO2 + H2O  : {%TrGTer} 1.72E-12; {&2419}
<G44230>  OH + IPRHOC03H     = IPRHOC03                    : {%TrGTer} 4.80E-12; {&2419}
<G44231>  C4PAN5 {+M}        = IPRHOC03 + NO2              : {%TrGTer} K_PAN_M; {&2419}
<G44232>  C4PAN5 + OH        = CH3COCH3 + CO + NO2         : {%TrGTer} 4.75E-13; {&2419}
<G44233a> MB000              = IPRHOC02H                   : {%TrGTer} 1.60E-17*C(ind_H20)*(0.08+0.15); {&2419, 3031}
<G44233b> MB000              = IBUTALOH + H2O2             : {%TrGTer} 1.60E-17*C(ind_H20)*0.77; {&2419, 3031}
<G44234>  MB000 + CO         = IBUTALOH + CO2              : {%TrGTer} 1.20E-15; {&2419}
<G44235>  MB000 + NO         = IBUTALOH + NO2              : {%TrGTer} 1.00E-14; {&2419}
<G44236>  MB000 + NO2        = IBUTALOH + NO3              : {%TrGTer} 1.00E-15; {&2419}
<G44400>  MALANHY    + OH  = MALANHYO2                   : {%TrGAro} 1.4E-12; {&2419}
<G44401a> MALDIALOOH + OH  = HOCOC4DIAL + OH             : {%TrGAro} 1.22E-10; {&2419}
<G44401b> MALDIALOOH + OH  = MALDIAL02                   : {%TrGAro} 0.6*k_CH300H_OH; {&2419}
<G44402>  NC4DC02H   + OH  = MALANHY + NO2               : {%TrGAro} 0.6*k_CH300H_OH; {&2419} // KDEC NC4DC02$\rightarrow$ MALANHY + NO2
<G44403>  C01403C02H + OH  = HCOCH202 + 2 CO2            : {%TrGAro} 2.19E-11; {&2419}
<G44404>  BZFU00H    + OH  = BZFU02                      : {%TrGAro} 3.68E-11; {&2419}
<G44405>  HOCOC4DIAL + OH  = CO2C4DIAL + HO2             : {%TrGAro} 3.67E-11; {&2419}
<G44406a> MALDIALC03 + HO2 = MALDALC02H + O3             : {%TrGAro} KAPH02*rco3_o3; {&2419}
<G44406b> MALDIALC03 + HO2 = MALDALC03H                  : {%TrGAro} KAPH02*rco3_ooh; {&2419}
<G44406c> MALDIALC03 + HO2 = .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2 + OH  : {%TrGAro} KAPH02*rco3_oh; {&2419} // KDEC MALDIALC02 $\rightarrow$ .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2
<G44407>  MALDIALC03 + NO  = .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2 + NO2 : {%TrGAro} KAPNO; {&2419} // KDEC MALDIALC02 $\rightarrow$ .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2
<G44408>  MALDIALC03 + NO2 = MALDIALPAN                          : {%TrGAro} k_CH3C03_NO2; {&2419}
<G44409>  MALDIALC03 + NO3 = .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2 + NO2 : {%TrGAro} KR02NO3*1.74; {&2419} // KDEC MALDIALC02 $\rightarrow$ .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2
<G44410>  MALDIALC03       = .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2       : {%TrGAro} k1_R02RC03; {&2419} // KDEC MALDIALC02 $\rightarrow$ .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2
<G44411>  BZFUONE    + NO3 = NBZFU02                     : {%TrGAro} 3.00E-13; {&2419}
<G44412>  BZFUONE    + O3  = .3125 C01403C02H + .1875 C01403CHO + .1875 H202 + .5 CO + .5 CO2 + .5 HCOCH202 + .5 OH : {%TrGAro} 2.20E-19;// KDEC BZFU0N00A $\rightarrow$    .5 BZFU0N00 + .5 CO + .5 CO2 + .5
HCOCH202 + .5 OH and BZFU0N00 $\rightarrow$ .625 C01403C02H + .375 C01403CHO + .375 H202
<G44413>  BZFUONE    + OH  = BZFU02                      : {%TrGAro} 4.45E-11; {&2419}
<G44414>  NBZFU00H   + OH  = NBZFU02                     : {%TrGAro} 6.18E-12; {&2419}
<G44415>  MALDALC03H + OH  = MALDIALC03                  : {%TrGAro} 4.00E-11; {&2419}
<G44416>  EPXDLC02H  + OH  = C3DIAL02 + CO2              : {%TrGAro} 2.31E-11; {&2419}
<G44417a> EPXDLC03   + HO2 = C3DIAL02 + CO2 + OH         : {%TrGAro} KAPH02*rco3_oh; {&2419}
<G44417b> EPXDLC03   + HO2 = EPXDLC02H + O3              : {%TrGAro} KAPH02*rco3_o3; {&2419}
<G44417c> EPXDLC03   + HO2 = EPXDLC03H                   : {%TrGAro} KAPH02*rco3_ooh; {&2419}
<G44418>  EPXDLC03   + NO  = C3DIAL02 + CO2 + NO2        : {%TrGAro} KAPNO; {&2419}
<G44419>  EPXDLC03   + NO2 = EPXDLPAN                    : {%TrGAro} k_CH3C03_NO2; {&2419}
<G44420>  EPXDLC03   + NO3 = C3DIAL02 + CO2 + NO2        : {%TrGAro} KR02NO3*1.74; {&2419}
<G44421>  EPXDLC03         = C3DIAL02 + CO2              : {%TrGAro} k1_R02RC03; {&2419} // Only major channel.
<G44422>  MALNHYOHCO + OH  = CO + CO + CO + CO2 + HO2    : {%TrGAro} 5.68E-12; {&2419}
<G44423>  MALDIAL    + NO3 = MALDIALC03 + HNO3           : {%TrGAro} 2*KNO3AL*2.0; {&2419}
<G44424>  MALDIAL    + O3  =  1.0675 GLYOX + .1125 HCHO + .1125 HCOCO2H + .0675 H2O2  + .82 HO2 + .57 OH + 1.265 CO + .25 CO2 : {%TrGAro} 2.00E-18; {&2419} // KDEC: GLY00A $\rightarrow$    .125 HCHO + .18
GLY00 + 0.82 HO2 + .57 OH + 1.265 CO + .25 CO2 and H20 substitution GLY00 $\rightarrow$ .625 HCOCO2H + .375 GLYOX + .375 H2O2
<G44425>  MALDIAL    + OH  = .83 MALDIALC03 + .17 MALDIAL02 : {%TrGAro} 5.20E-11; {&2419} // Merged equations.
<G44426>  MALANHY00H + OH  = MALNHYOHCO + OH             : {%TrGAro} 4.66E-11; {&2419}
<G44427>  MALDIALPAN + OH  = GLYOX + CO + CO + NO2       : {%TrGAro} 3.70E-11; {&2419}
<G44428>  MALDIALPAN       = MALDIALC03 + NO2            : {%TrGAro} k_PAN_M; {&2419}
<G44429a> MALANHY02  + HO2 = MALANHY00H                  : {%TrGAro} KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh); {&2419, 3031}
<G44429b> MALANHY02  + HO2 = HCOCOHCO3 + CO2 + OH        : {%TrGAro} KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh); {&2419, 3031}
<G44430>  MALANHY02  + NO  = HCOCOHCO3 + CO2 + NO2       : {%TrGAro} KR02NO; {&2419} // KDEC MALANHYO $\rightarrow$ HCOCOHCO3
<G44431>  MALANHY02  + NO3 = HCOCOHCO3 + CO2 + NO2       : {%TrGAro} KR02NO3; {&2419} // KDEC MALANHYO $\rightarrow$ HCOCOHCO3
<G44432>  MALANHY02        = HCOCOHCO3 + CO2             : {%TrGAro} k1_R02s0R02; {&2419} // Only major channel. KDEC MALANHYO $\rightarrow$ HCOCOHCO3
<G44433>  EPXDLC03H  + OH  = EPXDLC03                    : {%TrGAro} 2.62E-11; {&2419}
<G44434>  CO2C4DIAL  + OH  = CO + CO + CO + CO + HO2     : {%TrGAro} 2.45E-11; {&2419}
<G44435a> NBZFU02    + HO2 = NBZFU00H                    : {%TrGAro} KR02H02(4)*(1-rcoch2o2_oh); {&2419, 3031}
<G44435b> NBZFU02    + HO2 = .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2 + OH  : {%TrGAro} KR02H02(4)*rcoch2o2_oh; {&2419, 3031}
<G44436>  NBZFU02    + NO  = .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2 + NO2 : {%TrGAro} KR02NO; {&2419} // KDEC NBZFU0 $\rightarrow$ .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2
<G44437>  NBZFU02    + NO3 = .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2 + NO2 : {%TrGAro} KR02NO3; {&2419} // KDEC NBZFU0 $\rightarrow$ .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2
<G44438>  NBZFU02          = .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2       : {%TrGAro} k1_R02s0R02; {&2419} // KDEC NBZFU0 $\rightarrow$ .5 C01403CHO + .5 NO2 + .5 NBZFUONE + .5 HO2 and R02 Only major
channel.
<G44439>  MALDALC02H + OH  = .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2       : {%TrGAro} 3.70E-11; {&2419} // KDEC MALDIALC02 $\rightarrow$ .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2
<G44440>  EPXC4DIAL  + NO3 = EPXDLC03 + HNO3             : {%TrGAro} 2*KNO3AL*4.0; {&2419}
<G44441>  EPXC4DIAL  + OH  = EPXDLC03                    : {%TrGAro} 4.32E-11; {&2419}
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<G44442a> MEC0ACET02 + H02 = MEC0ACE00H                : {%TrGAro} KR02H02(4)*(1-rcoch2o2_oh); {&2419, 3031}
<G44442b> MEC0ACET02 + H02 = CH3CO3 + HCH0 + C02 + 0H  : {%TrGAro} KR02H02(4)*rcoch2o2_oh; {&2419, 3031}
<G44443>  MEC0ACET02 + N0  = CH3CO3 + HCH0 + C02 + N02 : {%TrGAro} KR02N0; {&2419} // KDEC MEC0ACET0 $\rightarrow$ CH3CO3 + HCH0
<G44444>  MEC0ACET02 + N03 = CH3CO3 + HCH0 + C02 + N02 : {%TrGAro} KR02N03; {&2419} // KDEC MEC0ACET0 $\rightarrow$ CH3CO3 + HCH0
<G44445>  MEC0ACET02       = CH3CO3 + HCH0 + C02       : {%TrGAro} k1_R02p0R02; {&2419} // KDEC MEC0ACET0 $\rightarrow$ CH3CO3 + HCH0
<G44446>  C01403CH0  + N03 = C0 + HC0CH202 + C02 + HN03 : {%TrGAro} KN03AL*8.0; {&2419}
<G44447>  C01403CH0  + 0H  = C0 + HC0CH202 + C02        : {%TrGAro} 3.44E-11; {&2419}
<G44448>  NBZFU0NE   + 0H  = BZFUC0 + N02               : {%TrGAro} 1.16E-12; {&2419}
<G44449a> BZFU02     + H02 = BZFU00H                   : {%TrGAro} KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh); {&2419, 3031}
<G44449b> BZFU02     + H02 = C01403CH0 + H02 + 0H      : {%TrGAro} KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh); {&2419, 3031}
<G44450>  BZFU02     + N0  = C01403CH0 + H02 + N02     : {%TrGAro} KR02N0; {&2419} // KDEC BZFU0 $\rightarrow$ C01403CH0 + H02
<G44451>  BZFU02     + N03 = C01403CH0 + H02 + N02     : {%TrGAro} KR02N03; {&2419} // KDEC BZFU0 $\rightarrow$ C01403CH0 + H02
<G44452>  BZFU02           = C01403CH0 + H02           : {%TrGAro} k1_R02s0R02; {&2419} // KDEC BZFU0 $\rightarrow$ C01403CH0 + H02. Only major channel.
<G44453>  BZFUC0     + 0H  = C01403CH0 + H02           : {%TrGAro} 1.78E-11; {&2419}
<G44454a> MALDIAL02  + H02 = MALDIAL00H                : {%TrGAro} KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh); {&2419}
<G44454b> MALDIAL02  + H02 = GLY0X + GLY0X + H02 + 0H  : {%TrGAro} KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh); {&2419}
<G44457>  MALDIAL02  + N0  = GLY0X + GLY0X + H02 + N02 : {%TrGAro} KR02N0; {&2419} // KDEC MALDIAL0 $\rightarrow$ GLY0X + GLY0X + H02
<G44458>  MALDIAL02  + N03 = GLY0X + GLY0X + H02 + N02 : {%TrGAro} KR02N03; {&2419} // KDEC MALDIAL0 $\rightarrow$ GLY0X + GLY0X + H02
<G44459>  MALDIAL02        = GLY0X + GLY0X + H02       : {%TrGAro} k1_R02s0R02; {&2419} // KDEC MALDIAL0 $\rightarrow$ GLY0X + GLY0X + H02. Only major channel.
<G44460>  EPXDLPAN   + 0H  = C33C0 + C0 + N02          : {%TrGAro} 2.29E-11; {&2419}
<G44461>  EPXDLPAN         = EPXDLC03 + N02            : {%TrGAro} k_PAN_M; {&2419} // KBPAN $\rightarrow$ k\_PAN\_M
<G44462>  MEC0ACE00H + 0H  = MEC0ACET02                : {%TrGAro} 3.59E-12; {&2419}
<G45000>  C5H8      + 03   = .3508 MACR + .01518 MAC02H + .2440 MVK + .7085 HCH0  + .11 CH200 + .1275 C3H6 + .1575 CH3C0 + .0510 CH3  + .2625 H02 + .27 0H + .09482 H202 + .255 C02 + .522 C0 + .07182 HCH0 +
.03618 HC0CH202 + .01782 C0 + 0.05408 LCARB0N : {%TrG} 1.03E-14*EXP(-1995./temp); {&1759, 3031}
<G45001>  C5H8      + 0H   = .63 IS0PAB + .30 IS0PCD + .07 LIS0PEF02     : {%TrG} 2.7E-11*EXP(390./temp); {&1759, 3031}
<G45002>  C5H8      + N03  = NIS0P02     : {%TrG} 3.0E-12*EXP(-450./temp); {&1759}
<G45003a> IS0PAB    + 02   = LIS0PAC02   : {%TrG} 5.53DE-13; {&3031}
<G45003b> IS0PAB    + 02   = IS0PB02     : {%TrG} 3.E-12; {&3031}
<G45004a> IS0PCD    + 02   = LDIS0PAC02  : {%TrG} 6.78DE-13; {&3031}
<G45004b> IS0PCD    + 02   = IS0PD02     : {%TrG} 3.E-12; {&3031}
<G45005>  LIS0PAC02        = IS0PAB + 02 : {%TrG} 3.1E12*exp(-7900./temp)*.6+7.8E13*exp(-8600./temp)*.4; {&3031}
<G45006>  IS0PB02          = IS0PAB + 02 : {%TrG} 3.7E14*exp(-9570./temp)+4.2E14*exp(-9970./temp); {&3031}
<G45007>  LDIS0PAC02       = IS0PCD + 02 : {%TrG} 5.65E12*exp(-8410./temp)*.42+1.4E14*exp(-9110./temp)*.58; {&3031}
<G45008>  IS0PD02          = IS0PCD + 02 : {%TrG} 5.0E14*exp(-10120./temp)+8.25E14*exp(-10220/temp); {&3031}
<G45009a> LIS0PAC02        = C10DC202C400H       : {%TrG} K16HSZ14 * 2./3.*(1-fhpal); {&3031} {Approx. it should be C10DC202C300HC400H}
<G45009b> LIS0PAC02        = ZC0DC23DBC00H + H02  : {%TrG} K16HSZ14 * (2./3.*fhpal + 1./3.); {&3031}
<G45010a> LDIS0PAC02       = C100HC302C40D       : {%TrG} k16HSZ41 * 2./3.*(1-fhpal); {&3031} {Approx., it should be C100HC200HC302C40D}
<G45010b> LDIS0PAC02       = ZC0DC23DBC00H + H02  : {%TrG} k16HSZ41 * (2./3.*fhpal + 1./3.); {&3031}
<G45011>  LIS0PAC02        = .9 LIS0PAC0 + .1 IS0PA0H                                : {%TrG} k1_R02LIS0PAC02; {&2419, 3031}
<G45012>  LIS0PAC02  + H02 = LIS0PAC00H                                              : {%TrG} KR02H02(5); {&2419}
<G45013a> LIS0PAC02  + N0  = LIS0PAC0 + N02                                          : {%TrG} KR02N0*(1.-alpha_AN(6,1,0,0,0,temp,cair)); {&3158, 3159, 3031}
<G45013b> LIS0PAC02  + N0  = LIS0PACN03                                              : {%TrG} KR02N0*alpha_AN(6,1,0,0,0,temp,cair); {&3158, 3159, 3031}
<G45014>  LIS0PAC02  + N03 = LIS0PAC0 + N02                                          : {%TrG} KR02N03; {&2419}
<G45015>  LDIS0PAC02       = .9 LDIS0PAC0 + .1 IS0PA0H                               : {%TrG} k1_R02LIS0PAC02; {&2419, 3031}
<G45016>  LDIS0PAC02 + H02 = LIS0PAC00H                                              : {%TrG} KR02H02(5); {&2419}
<G45017a> LDIS0PAC02 + N0  = LDIS0PAC0 + N02                                         : {%TrG} KR02N0*(1.-alpha_AN(6,1,0,0,0,temp,cair)); {&3158, 3159, 3031}
<G45017b> LDIS0PAC02 + N0  = LIS0PACN03                                              : {%TrG} KR02N0*alpha_AN(6,1,0,0,0,temp,cair); {&3158, 3159, 3031}
<G45018>  LDIS0PAC02 + N03 = LDIS0PAC0 + N02                                         : {%TrG} KR02N03; {&2419}
<G45019a> LIS0PAC00H + 0H  = LIS0PAC02                                               : {%TrG} 0.6*k_CH300H_0H; {&3031}
<G45019b> LIS0PAC00H + 0H  = ZC0DC23DBC00H + H02                                     : {%TrG} k_s*f_allyl*f_soh; {&3031}
<G45019c> LIS0PAC00H + 0H  = LHC4ACCH0 + 0H                                          : {%TrG} (k_s*f_sooh*f_allyl+ k_rohro); {&3031}
<G45019d> LIS0PAC00H + 0H  = LIEP0X + 0H                                             : {%TrG} (k_adt+k_ads)*a_ch2oh*a_ch2ooh; {&3031} // Delta-1 and delta-2 LIEP0X are not considered and replaced by beta-
LIEP0X formed by IS0PB00H and IS0PD00H.
<G45020>  IS0PA0H    + 0H  = LHC4ACCH0 + H02                                         : {%TrG} (k_adt+k_ads)*a_ch2oh*a_ch2oh+k_s*f_soh*f_allyl+k_rohro; {&3031}
<G45021>  LIS0PACN03 + 0H  = LIS0PACN0302                                            : {%TrG} (k_adt+k_ads)*a_ch2ono2*a_ch2oh; {&3031} // SAR estimate within uncertainty range of the experimentally
determined rate constant by \citet{2093}, 1.1E-11.
<G45022>  IS0PB02          = .8 MVK + .8 HCH0 + .8 H02 + .2 IS0PB0H                  : {%TrG} k1_R02IS0PB02; {&2419}
<G45023a> IS0PB02    + H02 = IS0PB00H                                                : {%TrG} KR02H02(5)*(1.-rchohch2o2_oh); {&3031}
<G45023b> IS0PB02    + H02 = MVK + HCH0 + H02 + 0H                                   : {%TrG} KR02H02(5)*rchohch2o2_oh; {&3031}
<G45024a> IS0PB02    + N0  = MVK + HCH0 + H02 + N02                                  : {%TrG} KR02N0*(1.-alpha_AN(6,3,0,0,0,temp,cair)); {&3158, 3031}
<G45024b> IS0PB02    + N0  = IS0PBN03                                                : {%TrG} KR02N0*alpha_AN(6,3,0,0,0,temp,cair); {&3158, 3031}
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<G45025>  ISOPBO2    + NO3 = MVK + .75 HCHO + .75 HO2 + .25 CH3 + NO2                : {%TrG} KRO2NO3; {&2419}
<G45026a> ISOPBOOH + OH    = LIEPOX + OH                                           : {%TrG} (k_ads+k_adp)*a_ch2ooh; {&3151, 3031}
<G45026b> ISOPBOOH + OH    = ISOPBO2                                               : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G45026c> ISOPBOOH + OH    =  MGLYOX + HOCH2CHO                                    : {%TrG} k_rohro+k_s*f_alk*f_soh; {&3031}
<G45027>  ISOPBOOH + O3    = .1368 MACROOH + .1368 H2O2 + .2280 HO2 + .4332 ACETOL + .2280 CO2 + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 HO2 + .06880 OH + .2709 CO + .1591 CH2OO    : {%TrG}
1.E-17; {&3031}
<G45028>  ISOPBOH  + OH    = MVK + .75 HCHO + .75 HO2 + .25 CH3                    : {%TrG} k_s*f_alk*f_soh+(k_adp+k_ads)*a_ch2oh; {&3031}
<G45029>  ISOPBNO3   + OH  = ISOPBDNO3O2                                           : {%TrG} (k_adt+k_adp)*f_ch2ono2; {&3031}
<G45030>  ISOPDO2          = .8 MACR + .8 HCHO + .8 HO2 + .1 HCOCO + .1 ISOPDOH    : {%TrG} k1_RO2ISOPDO2; {&2419}
<G45031a> ISOPDO2    + HO2 = ISOPDOOH                                              : {%TrG} KRO2HO2(5)*(1.-rchohch2o2_oh); {&3031}
<G45031b> ISOPDO2    + HO2 = MACR + HCHO + HO2 + OH                                : {%TrG} KRO2HO2(5)*rchohch2o2_oh; {&3031}
<G45032a> ISOPDO2    + NO  = MACR + HCHO + HO2 + NO2                               : {%TrG} KRO2NO*(1.-alpha_AN(6,2,0,0,0,temp,cair)); {&3158, 3031}
<G45032b> ISOPDO2    + NO  = ISOPDNO3                                              : {%TrG} KRO2NO*alpha_AN(6,2,0,0,0,temp,cair); {&3158, 3031}
<G45033>  ISOPDO2    + NO3 = MACR + HCHO + HO2 + NO2                               : {%TrG} KRO2NO3; {&2419}
<G45034a> ISOPDOOH   + OH  = LIEPOX + OH                                           : {%TrG} (k_adt+k_adp)*a_ch2ooh; {&3151, 3031}
<G45034b> ISOPDOOH   + OH  = ISOPDO2                                               : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G45034c> ISOPDOOH   + OH  = HCOCO + OH                                            : {%TrG} k_t*f_tooh*f_allyl*f_pch2oh; {&3031}
<G45034d> ISOPDOOH   + OH  = ACETOL + GLYOX + OH                                   : {%TrG} k_s*f_pch2oh*f_soh; {&3031}
<G45035>  ISOPDOOH   + O3  = 1.393 OH + BIACETOH + .67 HCHO + .05280 HO2 + .2079 CO + .1221 CH2OO  : {%TrG} 1.E-17; {&3031}
<G45036>  ISOPDOH    + OH  = HCOCO + HO2                                           : {%TrG} 2.*k_rohro+(k_t*f_toh*f_allyl+k_s*f_soh)*f_pch2oh+(k_adt+k_adp)*a_ch2oh; {&3031}
<G45037>  ISOPDNO3   + OH  = ISOPBDNO3O2                                           : {%TrG} (k_adp+k_ads)*a_ch2ono2; {&3031} // SAR estimate within uncertainty range of the experimentally determined rate
constant by \citet{2093}, 4.2E-11.
<G45038>  NISOPO2          = .8 NC4CHO + .6 HO2 + .2 LISOPACNO3                    : {%TrG} k1_RO2LISOPACO2; {&2419}
<G45039>  NISOPO2    + HO2 = NISOPOOH                                              : {%TrG} KRO2HO2(5); {&2419}
<G45040>  NISOPO2    + NO  = NC4CHO + HO2 + NO2                                    : {%TrG} KRO2NO; {&2419} // \alkylnitrateneglected
<G45041>  NISOPO2    + NO3 = NC4CHO + HO2 + NO2                                    : {%TrG} KRO2NO3; {&2419}
<G45042>  NISOPOOH   + OH  = NC4CHO + OH                                           : {%TrG} 1.03E-10; {&2419}
<G45043>  NC4CHO     + OH  = LNISO3                                                : {%TrG} (k_adt+k_ads)*a_cho*a_ch2ono2; {&3031} // Old MCM rate constant 4.16E-11.
<G45044>  NC4CHO     + O3  = .27 NOA + .027 HCOCO2H + .0162 GLYOX + .0162 H2O2 + .1458 HCOCO + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 NO2 + 0.7705 HCHO + .4055 CO2 + .73 GLYOX  : {%TrG}
2.40E-17; {&3031}
<G45045>  NC4CHO     + NO3 = LNISO3 + HNO3                                         : {%TrG} KNO3AL*4.25; {&2419}
<G45046>  LNISO3     + HO2 = LNISOOH                                               : {%TrG} .5*KRO2HO2(5) + .5*KAPHO2; {&2419}
<G45047>  LNISO3     + NO  = NOA + .5 HOCHCHO + .5 CO + .5 HO2 + NO2 + .5 CO2      : {%TrG} .5*KAPNO +.5*KRO2NO; {&2419} // \alkylnitrateneglected
<G45048>  LNISO3     + NO3 = NOA + .5 HOCHCHO + .5 CO + .5 HO2 + NO2 + .5 CO2      : {%TrG} 1.3*KRO2NO3; {&2419}
<G45049>  LNISOOH    + OH  = LNISO3                                                : {%TrG} 2.65E-11; {&2419}
<G45050a> LHC4ACCHO  + OH  = LC57802                                               : {%TrG} (k_adtertprim+k_ads)*a_cho*a_ch2oh; {&3031}
<G45050b> LHC4ACCHO  + OH  = LHC4ACCO3                                             : {%TrG} k_t*f_o; {&3031}
<G45050c> LHC4ACCHO  + OH  = ZCODC23DBCOD + HO2                                    : {%TrG} k_s*f_soh*f_allyl; {&3031}
<G45051>  LHC4ACCHO  + O3  = .2225 CH3CO + .89 CO + .01171875 HOCH2CO2H + .075625 H2O2 + .01171875 HCOCO2H + .2775 ACETOL + .6675 HO2 + .2603125 GLYOX + .2225 HCHO + .89 OH + .2603125 HOCH2CHO + .5 MGLYOX   :
{%TrG} 2.40E-17; {&2419}
<G45052>  LHC4ACCHO  + NO3 = LHC4ACCO3 + HNO3                                      : {%TrG} KNO3AL*4.25; {&2419}
<G45053>  LC57802          = .25 ACETOL + .75 MGLYOX + .25 HOCHCHO + .75 HOCH2CHO + .75 HO2 : {%TrG} k1_RO2TORO2; {&2419}
<G45054a> LC57802    + HO2 = MGLYOX + HOCH2CHO + OH                                : {%TrG} KRO2HO2(5)*rcoch2o2_oh; {&2419}
<G45054b> LC57802    + HO2 = LC57800H                                              : {%TrG} KRO2HO2(5)*rcoch2o2_ooh; {&2419}
<G45055>  LC57802    + NO  = .25 ACETOL + .75 MGLYOX + .25 HOCHCHO + .75 HOCH2CHO + .75 HO2 + NO2 : {%TrG} KRO2NO; {&2419} // \alkylnitrateneglected
<G45056>  LC57802    + NO3 = .25 ACETOL + .75 MGLYOX + .25 HOCHCHO + .75 HOCH2CHO + .75 HO2 + NO2 : {%TrG} KRO2NO3; {&2419}
<G45057>  LC57802          = .25 ACETOL + .75 MGLYOX + .25 HOCH2CHO + .75 HOCH2CHO + HO2 + OH       : {%TrG} KHSB; {&3031}
<G45058a> LC57800H   + OH = LC57802                                               : {%TrG} 0.6*k_CH3OOH_OH; {&3031}
<G45058b> LC57800H   + OH = C10DC200HC40D + HO2                                   : {%TrG} k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_pch2oh*f_pch2oh+k_s*f_soh*f_pch2oh; {&3031}
<G45059a> LHC4ACCO3        = OH + .5 MACRO2 + .5 LHMVKABO2 + CO2                   : {%TrG} k1_RO2RCO3*0.9; {&3031}
<G45059b> LHC4ACCO3        = LHC4ACCO2H                                            : {%TrG} k1_RO2RCO3*0.1; {&3031}
<G45060a> LHC4ACCO3  + HO2 = 2 OH + .5 MACRO2 + .5 LHMVKABO2 + CO2                 : {%TrG} KAPHO2*rco3_oh; {&3031}
<G45060b> LHC4ACCO3  + HO2 = LHC4ACCO3H                                            : {%TrG} KAPHO2*rco3_ooh; {&3031}
<G45060c> LHC4ACCO3  + HO2 = LHC4ACCO2H + O3                                       : {%TrG} KAPHO2*rco3_o3; {&3031}
<G45061>  LHC4ACCO3  + NO  = .5 MACRO2 + .5 LHMVKABO2 + NO2  + CO2                : {%TrG} KAPNO; {&3031}
<G45062>  LHC4ACCO3  + NO2 = LC5PAN1719                                            : {%TrG} k_CH3CO3_NO2; {&2419}
<G45063>  LHC4ACCO3  + NO3 = .5 MACRO2 + .5 LHMVKABO2 + NO2  + CO2                : {%TrG} 1.6*KRO2NO3; {&3031}
<G45064a> LHC4ACCO2H + OH  = OH + .5 MACRO2 + .5 LHMVKABO2  + CO2                  : {%TrG} 2.52E-11; {&3031}
<G45064b> LHC4ACCO3H + OH  = LHC4ACCO3                                             : {%TrG} 2.88E-11; {&2419}
<G45065>  LC5PAN1719       = LHC4ACCO3 + NO2                                       : {%TrG} k_PAN_M; {&2419}
<G45066>  LC5PAN1719 + OH  = .5 MACROH + .5 HO12CO3C4 + CO + NO2                   : {%TrG} 2.52E-11; {&2419}
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<G45067>  HC0C5      + 0H  = C5902                                                    : {%TrG} 3.81E-11; {&2419}
<G45068>  HC0C5      + 03  = BIACET0H + .335 H202 + .67 HCH0 + .2079 C0 + .1221 CH200 + .05280 0H   : {%TrG} 7.51E-16*EXP(-1521./temp); {&3031}
<G45069>  C5902            = ACET0L + H0CH2C0                                       : {%TrG} k1_R02t0R02; {&3031}
<G4507Oa> C5902      + H02 = 0H + ACET0L + H0CH2C0                                  : {%TrG} KR02H02(5)*rcoch2o2_oh; {&3031}
<G4507Ob> C5902      + H02 = C5900H                                                 : {%TrG} KR02H02(5)*rcoch2o2_ooh; {&3031}
<G45071>  C5902      + N0  = ACET0L + H0CH2C0 + N02                                 : {%TrG} KR02N0; {&3031} // \alkylnitrateneglected
<G45072>  C5902      + N03 = ACET0L + H0CH2C0 + N02                                 : {%TrG} KR02N03; {&3031}
<G45073>  C5900H     + 0H  = C5902                                                  : {%TrG} 9.7E-12; {&2419}
<G45074>  LIEP0X     + 0H  = DB10 + H20                                             : {%TrG} 5.78E-11*EXP(-400./temp)*(1.52/3.+0.98*2./3.)/1.51; {&3151, 3178, 3031} // Formic acid production consistent
with results of \citet{3178}. Here, the high yields of formic acid and hydroxycarbonyls at low N0 from oxidation of cis-beta-LIEP0X (the most abundant isomer) are approximated with the production of DB10
which undergo both the Dibble double H-transfer to DB202 and H0CH2 elimination yielding \kpp{HVMK} and \kpp{HMAC} (keto-vinyl alcohol potentially arising from decomposition of the alkoxy radical resulting
from the ring opening after H-abstraction). The rate constant is from \citet{3151} and adjusted based on \citet{3178} that determined the single rate constants for the cis- and trans- beta isomer.
<G45075>  IS0PB02          = MVK + HCH0 + 0H                                        : {%TrG} KHSB; {&3031}
<G45076>  IS0PD02          = MACR + HCH0 + 0H                                       : {%TrG} KHSD; {&3031}
<G45077a> ZC0DC23DBC00H + 0H = .6 C10DC202C400H + .4 C100HC202C40D                  : {%TrG} k_adt*a_cho*a_ch2ooh; {&3031}
<G45077b> ZC0DC23DBC00H + 0H = .6 C10DC302C400H + .4 C100HC302C40D                  : {%TrG} k_ads*a_cho*a_ch2ooh; {&3031}
<G45077c> ZC0DC23DBC00H + 0H = ZC03HC23DBC0D                                       : {%TrG} k_t*f_o*f_alk+0.6*k_CH300H_0H; {&3031}
<G45077d> ZC0DC23DBC00H + 0H = ZC0DC23DBC0D + 0H                                   : {%TrG} k_s*f_sooh*f_allyl; {&3031}
<G45078>  ZC0DC23DBC00H + 03 = .4672 0H + .2336 CH0C0CH202 + .2336 C0 + .2336 CH3C0 + .4672 H00CH2CH0 + .1728 MGLY0X + .1901 0H + .0864 GLY0X + .02765 H00CH2CH0 + .02765 H202 + .02592 CH300H + .02592 C02 +
.01037 HC0C0 + .01555 CH200 + .01555 C0 + .006908 H00CH2C03 + .2628 0H + .1314 MGLY0X + .1314 0H + .1314 HC0C0CH200H + .2628 GLY0X + .0972 HYPERACET + .00972 HC0C02H + .005832 GLY0X + .005832 H202 + .05249
0H + .05249 HC0C0 + .01458 HCH0 + .01458 C02 + .01458 HC00H + .01458 C0  : {%TrG} 2.4E-17; {&3031}
<G45079>  C100HC202C40D        = .78 HYPERACET + .78 H0CHCH0 + .22 C02H3CH0 + .22 HCH0 + .22 0H          : {%TrG} k1_R02t0R02; {&3031}
<G4507A0> C100HC202C40D + N0   = .78 HYPERACET + .78 H0CHCH0 + .22 C02H3CH0 + .22 HCH0 + .22 0H + N02    : {%TrG} KR02N0; {&3031} // \alkylnitrateneglected
<G4507A1a> C100HC202C40D + H02  = C100HC200HC40D                                   : {%TrG} KR02H02(5)*rcoch2o2_ooh; {&3031}
<G4507A1b> C100HC202C40D + H02  = .78 HYPERACET + .78 H0CHCH0 + .22 C02H3CH0 + .22 HCH0 + 1.22 0H : {%TrG} KR02H02(5)*rcoch2o2_oh; {&3031}
<G4507A2> C100HC202C40D        = HYPERACET + GLY0X + 0H                          : {%TrG} KHSB; {&3031}
<G4507A3> C10DC202C400H        = 0H + C10DC200HC40D                              : {%TrG} K15HSDHB; {&3031}
<G4507A4a> C100HC200HC40D + 0H  = C10DC200HC40D + 0H                              : {%TrG} 2.*k_s*f_sooh*f_tch2oh; {&3031}
<G4507A4b> C100HC200HC40D + 0H  = HYPERACET + 2 C0 + 2 H02 + 0H                   : {%TrG} k_t*f_toh*f_pch2oh*f_pch2oh; {&3031}
<G4507A4c> C100HC200HC40D + 0H  = C100HC202C40D                                   : {%TrG} 0.6*k_CH300H_0H; {&3031}
<G4507A5> C10DC200HC40D  + 0H  = C02H3CH0 + C0 + H20 + 0H                         : {%TrG} k_t*f_o*f_tch2oh+k_t*f_toh*f_toh*f_cho; {&3031}
<G4507A6> C10DC302C400H        = MGLY0X + H00CH2CH0 + H02                        : {%TrG} k1_R02s0R02; {&3031}
<G4507A7> C10DC302C400H + N0   = MGLY0X + H00CH2CH0 + H02 + N02                  : {%TrG} KR02N0; {&3031}
<G4507A8> C10DC302C400H + H02  = .5 CH3C0 + .5 C0 + .5 MGLY0X + .5 H02 + H00CH2C03   : {%TrG} KR02H02(5); {&3031}
<G4507A9> C10DC302C400H        = MGLY0X + 0H + H00CH2CH0                         : {%TrG} KHSD; {&3031}
<G4507B0> C100HC302C40D        = .625 MGLY0X + 2 C0 + 1.625 H02 + .375 CH3C0 + .375 C02 + 0H : {%TrG} K15HSDHB; {&3031}
<G4507B1> LHC4ACC03            = ZC03HC23DBC0D + H02         : {%TrG} K16HS; {&3031}
<G4507B2a> ZC0DC23DBC0D + 0H    = C10DC202C40D               : {%TrG} (k_adt+k_ads)*a_cho*a_cho; {&3031} // ZC0DC23DBC0D = CM4DIAL in MCM only from aromatics.
<G4507B2b> ZC0DC23DBC0D + 0H    = ZC03C23DBC0D               : {%TrG} 2*k_t*f_o*f_alk; {&3031} // Only one acyl peroxy radical considered.
<G4507B3> ZC0DC23DBC0D + N03   = ZC03C23DBC0D + HN03        : {%TrG} KN03AL*4.25*2.; {&3031} // Two aldehydic sites reacting with \kpp{N03} but only one isomer product considered.
<G4507B4a> C10DC202C40D + H02   = 0H + MGLY0X + H0CHCH0      : {%TrG} KR02H02(5)*rcoch2o2_oh; {&3031}
<G4507B4b> C10DC202C40D + H02   = C10DC200HC40D              : {%TrG} KR02H02(5)*rcoch2o2_ooh; {&3031}
<G4507B5> C10DC202C40D + N0    = N02 + MGLY0X + H0CHCH0      : {%TrG} KR02N0; {&3031} // \alkylnitrateneglected
<G4507B6> C10DC202C40D         = MGLY0X + H0CHCH0            : {%TrG} k1_R02t0R02; {&3031}
<G4507B7a> C10DC200HC40D + 0H   = MGLY0X + 2 C0              : {%TrG} (2.*k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_cho*f_pch2oh)*.5; {&3031}
<G4507B7b> C10DC200HC40D + 0H   = MGLY0X + 2 C0 + 0H         : {%TrG} (2.*k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_cho*f_pch2oh)*.5; {&3031}
<G4507B8> LIS0PACN0302 + N0    = .21 N0A + .21 H0CH2CH0 + .21 H02 + .49 H012C03C4 + .49 HCH0 + .49 N02 + .045 MVKN03 + .045 HCH0 + .255 ACET0L + .255 N03CH2CH0 + .225 H202 + N02 : {%TrG} KR02N0; {&3031} //
\alkylnitrateneglected
<G4507B9> LIS0PACN0302         = .21 N0A + .21 H0CH2CH0 + .21 H02 + .49 H012C03C4 + .49 HCH0 + .49 N02 + .045 MVKN03 + .045 HCH0 + .255 ACET0L + .255 N03CH2CH0 + .225 H202 : {%TrG}
k1_R02t0R02+KR02H02(5)*c(ind_H02); {&3031}
<G4510C0> IS0PBDN0302 + N0     = .6 ACET0L + .6 H0CH2CH0 + .26 MACRN + .14 MVKN03 + .4 HCH0 + .4 H02 + 1.6 N02 : {%TrG} KR02N0; {&3031} // \alkylnitrateneglected
<G4510D1> IS0PBDN0302          = .6 ACET0L + .6 H0CH2CH0 + .26 MACRN + .14 MVKN03 + .4 HCH0 + .4 H02 + .6 N02 : {%TrG} k1_R02s0R02+KR02H02(5)*c(ind_H02); {&3031}
<G4510E2> LIS0PACN03 + 03      = .8704 0H + .365 H02 + .73 MGLY0X + .4325 N03CH2CH0 + .135 ACET0L + .0675 GLY0X + .4325 N02 + .0891 H202 + .135 N0A + .0675 H0CHCH0 + .3866 H0CH2CH0 + .0405 CH30H + .0405 C0
+ .0054 H0CH2C0    : {%TrG} 2.8E-17; {&3157, 3031}
<G4510F3> DB102              = DB10                                                : {%TrG} k1_R02s0R02; {&3031}
<G4510Fa> DB102    + H02     = DB100H                                              : {%TrG} KR02H02(5)*(1.-rchohch2o2_oh); {&3031} // \kpp{DB100H} is a hydroperoxide bearing a vinyl alcohol
moiety that upon reaction with 0H yields HC00H \citep{2001}.
<G4510Fb> DB102    + H02     = DB10 + 0H                                           : {%TrG} KR02H02(5)*rchohch2o2_oh; {&3031}
<G4510Ga> DB102    + N0      = DB10 + N02                                          : {%TrG} KR02N0*(1.-alpha_AN(7,2,0,0,0,temp,cair)); {&3031}
<G4510Gb> DB102    + N0      = DB1N03                                              : {%TrG} KR02N0*alpha_AN(7,2,0,0,0,temp,cair); {&3031}
<G4510H> DB102    + N03     = DB10 + N02                                          : {%TrG} KR02N03; {&3031}
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<G45107>  DB102              = DB202 + OH                                                    : {%TrG} 1.E4; {&3181} // OH production here is to take into account the hydroperoxidic function formed by the shift of the enolic hydrogen and not present in DB202. This approximation leads to spurious \chem{HO_2} production.
<G45108a> DB10               = DB202                                                         : {%TrG} KDEC*0.72; // Consistent with the results of \citet{3178}.
<G45108b> DB10               = .5 HVMK + .5 HMAC + HCHO + HO2                                : {%TrG} KDEC*0.28; // Consistent with the results of \citet{3178}. Assuming that the enol alkoxy radical partly decomposes yielding a substitute vinyl alcohol.
<G45109>  DB202              = .48 ACETOL + .52 HOCH2CHO + .52 MGLYOX + .48 GLYOX + HO2      : {%TrG} k1_RO2s0RO2; {&3031}
<G45110a> DB202    + HO2     = DB200H                                                        : {%TrG} KR02H02(5)*(1.-rchohch2o2_oh); {&3031}
<G45110b> DB202    + HO2     = .48 ACETOL + .52 HOCH2CHO + .52 MGLYOX + .48 GLYOX + HO2 + OH : {%TrG} KR02H02(5)*rchohch2o2_oh; {&3031}
<G45111>  DB202    + NO      = .48 ACETOL + .52 HOCH2CHO + .52 MGLYOX + .48 GLYOX + HO2 + NO2 : {%TrG} KR02NO; // \alkylnitrateneglected
<G45112>  DB202    + NO3     = .48 ACETOL + .52 HOCH2CHO + .52 MGLYOX + .48 GLYOX + HO2 + NO2 : {%TrG} KR02NO3; {&3031}
<G45113>  DB202              = .48 MACROOH + .52 LHMVKABOOH + CO + OH                        : {%TrG} K14HSAL; {&3031}
<G45114a> DB100H   + OH      = DB102                                                         : {%TrG} .6*k_CH300H_OH; {&3031}
<G45114b> DB100H   + OH      = HCOOH + HO2 + CH3COCHO2CHO                                    : {%TrG} k_adt; {&3031} // Here, formic acid is mechanistically produced by the \chem{OH}-addition to the vinyl alcohol which, upon \chem{RO_2}-to-\chem{RO} conversion (skipped here), yields the HOCHOH fragment which in turn reacts with \chem{O_2} forming \chem{HCOOH + HO_2}. Along \chem{CH_3COCHOOHCHO} should be produced but not in the mechanism. Only \kpp{CH3COCHO2CHO}. The rate constant is consistent with predictions by \citet{2140} for \chem{ENOL}. OH-addition to the OH-bearing carbon is considered the dominant channel as it is already for the \chem{ENOL} \citep{2140}.
<G45115>  DB100H + HCOOH     = C10DC200HC40D  + HCOOH                                        : {%TrG} 4.67E-26*temp**3.286*EXP(4509./(1.987*temp)); {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}. The product should be C10DC300HC40D but it is neglected in the mechanism.
<G45116>  DB1NO3   + OH      = HCOOH + NO2 + CH3COCHO2CHO                                    : {%TrG} k_adt; {&3031} // As for DB100H + OH.
<G45117>  DB200H   + OH      = DB202                                                         : {%TrG} .6*k_CH300H_OH; {&3031} // Additional sinks for DB200H are neglected.
<G45118>  ISOPAC00H + O3 = 1.3272 OH + .36986 HO2 + .0432 H2O2 + .08422 CO + .2025 CH300H + .01215 CH200  + .3704 HCHO + .00405 CH3OH + .0405 CO2 + .1825 HOCH2COCHO2 + .365 MGLYOX + .3866 HOOCH2CHO + .135 ACETOL + .0675 GLYOX + .00324 HCOCO + .3866 HOCH2CHO + .135 HYPERACET  + .0675 HOCHCHO + .0054 HOCH2CO    : {%TrG} 4.829E-16; {&3031}
<G45119a> ZCO3HC23DBC0D + OH = .62 CO2H3CHO + .62 OH + .62 CO2 + .38 MGLYOX + .38 HCOCO3H + .38 HO2                    : {%TrG} k_adt*a_cho*a_co2h; {&3031}
<G45119b> ZCO3HC23DBC0D + OH = .62 CH3COCO3H + 1.24 CO + 1.24 HO2 + .38 MGLYOX + .38 HO2 + .38 CO + .38 HO2 + .38 OH + .38 CO2     : {%TrG} k_ads*a_cho*a_co2h; {&3031}
<G45120>  ISOPEF02         = ISOPEF0           : {%TrG} k1_RO2p0RO2; {&3031}
<G45121a> ISOPEF02 + NO    = ISOPEF0 + NO2     : {%TrG} KR02NO*(1.-alpha_AN(6,1,0,0,0,temp,cair)); {&3031}
<G45121b> ISOPEF02 + NO    = ISOPDNO3          : {%TrG} KR02NO*alpha_AN(6,1,0,0,0,temp,cair); {&3031} // Nitrate assumed to be major isomer that is mostly similar to products of ISOPD02-chemistry.
<G45122a> ISOPEF02 + HO2   = .7143 ISOPD00H + .2857 ISOPB00H     : {%TrG} KR02H02(5)*(1.-rchohch2o2_oh); {&3031}
<G45122b> ISOPEF02 + HO2   = ISOPEF0 + OH                        : {%TrG} KR02H02(5)*rchohch2o2_oh; {&3031}
<G45123>  ISOPEF02 + NO3   = ISOPEF0 + NO2                       : {%TrG} KR02NO3; {&3031}
<G45124>  ISOPEF02       = .7143 MACR + .2857 MVK + HCHO + OH   : {%TrG} .7143*KHSD+.2857*KHSB; {&3031}
<G45125>  ISOPEF0        = .7143 MACR + .2857 MVK + HCHO + HO2   : {%TrG} KDEC; {&3031}
<G45126a> ISOPAC0          = ME3FURAN + HO2                    : {%TrG} KDEC*0.37; {&3031, 3159, 3187}
<G45126b> ISOPAC0          = .65 LHC4ACCHO + .65 HO2 + .35 DB102       : {%TrG} KDEC*(1.-0.37); {&3031, 3159, 3187}
<G45127a> LDISOPAC0        = ME3FURAN + HO2                    : {%TrG} KDEC*0.37; {&3031, 3159, 3187}
<G45127b> LDISOPAC0        = .65 LHC4ACCHO + .65 HO2 + .35 DB102       : {%TrG} KDEC*(1.-0.37); {&3031, 3159, 3187}
<G45128>  ME3FURAN + OH = LME3FURAN02                       : {%TrG} 3.2E-11*EXP(310./temp); {&3031} // Rate constant by \citet{3206}. A lumped \chem{RO_2} that upon conversion to RO yields 100\% 2-methyl-butenedial (ZCODC23DBC0D) although \citet{3213} quantified a 38\% yield of the Z/E mixture.
<G45129>  ME3FURAN + NO3 = LME3FURAN02 + NO2             : {%TrG} 1.9E-11; {&3031, 1759} // As for 3METHYLFURAN + OH but with additional \chem{NO_2} production for mass conservation.
<G45130>  LME3FURAN02        = ZCODC23DBC0D + HO2            : {%TrG} k1_RO2s0RO2; {&3031}
<G45131>  LME3FURAN02 + NO   = ZCODC23DBC0D + HO2 + NO2      : {%TrG} KR02NO; {&3031} // \alkylnitrateneglected
<G45132>  LME3FURAN02 + HO2  = ZCODC23DBC0D + HO2            : {%TrG} KR02H02(5); {&3031} // Hydroperoxide formation neglected.
<G45133>  ZCO3C23DBC0D       = .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO2           : {%TrG} k1_RO2RC03; {&3031}
<G45134a> ZCO3C23DBC0D  + HO2 = .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO2 + OH      : {%TrG} KAPH02*rco3_oh; {&3031}
<G45134b> ZCO3C23DBC0D  + HO2 = ZCO3HC23DBC0D                                        : {%TrG} KAPH02*(rco3_ooh+rco3_o3); {&3031} // ZCO2HC23DBC0D formation is neglected. However, it is produced in MCM and in aromatic-related reactions under the name of MC30DBC02H.
<G45135>  ZCO3C23DBC0D  + NO  = .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO2 + NO2     : {%TrG} KAPNO; {&3031}
<G45136>  ZCO3C23DBC0D  + NO2 = ZCPANC23DBC0D                                        : {%TrG} k_CH3CO3_NO2; {&2419}
<G45137>  ZCO3C23DBC0D  + NO3 = .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO2 + NO2     : {%TrG} 1.6*KR02NO3; {&3031}
<G45138>  ZCPANC23DBC0D       = ZCO3C23DBC0D + NO2                                   : {%TrG} k_PAN_M; {&2419}
<G45139>  ZCPANC23DBC0D + OH  = .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO2 + NO2     : {%TrG} 2.52E-11; {&3031} // ZCPANC23DBC0D is assumed to react like LC5PAN1719.
<G45200>  C51102           = CH3CO + HCOCH2CHO              : {%TrGTer} k1_RO2s0RO2; {&2419}
<G45201>  C51102 + NO      = CH3CO + HCOCH2CHO + NO2        : {%TrGTer} KR02NO; {&2419} // \alkylnitrateneglected
<G45202a> C51102 + HO2     = C51100H                        : {%TrGTer} KR02H02(5)*rcoch2o2_ooh; {&2419, 3031}
<G45202b> C51102 + HO2     = CH3CO + HCOCH2CHO + OH         : {%TrGTer} KR02H02(5)*rcoch2o2_oh; {&2419, 3031}
<G45203>  C51100H + OH     = C51102                         : {%TrGTer} 7.49E-11; {&2419}
<G45204>  CO23C4CHO + OH   = CO23C4CO3                      : {%TrGTer} 6.65E-11; {&2419}
<G45205>  CO23C4CHO + NO3  = CO23C4CO3 + HNO3               : {%TrGTer} KNO3AL*5.5; {&2419}
<G45206>  CO23C4CO3        = BIACET02 + CO2                 : {%TrGTer} k1_RO2RC03; {&2419}
<G45207>  CO23C4CO3 + NO   = BIACET02 + CO2 + NO2           : {%TrGTer} KAPNO; {&2419} // \alkylnitrateneglected
<G45208>  CO23C4CO3 + NO2  = C5PAN9                         : {%TrGTer} k_CH3CO3_NO2; {&2419}
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<G45209a> C023C4C03 + H02  = C023C4C03H                      : {%TrGTer} KAPH02*(rco3_ooh+rco3_o3); {&2419}
<G45209b> C023C4C03 + H02  = BIACET02 + C02 + 0H             : {%TrGTer} KAPH02*rco3_oh; {&2419}
<G45210>  C5PAN9           = C023C4C03 + N02                 : {%TrGTer} k_PAN_M; {&2419}
<G45211>  C5PAN9 + 0H      = C023C3CH0 + C0 + N02            : {%TrGTer} 3.12E-13; {&2419}
<G45212>  C51202           = C51302                          : {%TrGTer} k1_R02pR02; {&2419}
<G45213>  C51202 + H02     = C51200H                         : {%TrGTer} KR02H02(5); {&2419}
<G45214>  C51202 + N0      = C51302 + N02                    : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G45215>  C51200H + 0H     = C013C4CH0 + 0H                  : {%TrGTer} 1.01E-10; {&2419}
<G45216>  C51302           = GLY0X + H0C2H4C03               : {%TrGTer} k1_R02s0R02; {&2419}
<G45217>  C51302 + N0      = GLY0X + H0C2H4C03 + N02         : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G45218a> C51302 + H02     = C51300H                         : {%TrGTer} KR02H02(5)*rcoch2o2_ooh; {&2419, 3031}
<G45218b> C51302 + H02     = GLY0X + H0C2H4C03 + 0H          : {%TrGTer} KR02H02(5)*rcoch2o2_oh; {&2419, 3031}
<G45219>  C013C4CH0 + 0H   = CH0C3C0C03                      : {%TrGTer} 1.33E-10; {&2419}
<G45220>  C013C4CH0 + N03  = CH0C3C0C03 + HN03               : {%TrGTer} 2.*KN03AL*5.5; {&2419}
<G45221>  C51300H + 0H     = C513C0 + 0H                     : {%TrGTer} 9.23E-11; {&2419}
<G45222>  CH0C3C0C03       = CH0C3C002 + C02                 : {%TrGTer} k1_R02RC03; {&2419}
<G45223>  CH0C3C0C03 + H02 = CH0C3C000H                      : {%TrGTer} KAPH02; {&2419}
<G45224>  CH0C3C0C03 + N02 = CH0C3C0PAN                      : {%TrGTer} k_CH3C03_N02; {&2419}
<G45225>  CH0C3C0C03 + N0  = CH0C3C002 + C02 + N02           : {%TrGTer} KAPN0; {&2419} // \alkylnitrateneglected
<G45226>  C513C0 + 0H      = H0C2H4C03 + C0 + C0             : {%TrGTer} 2.64E-11; {&2419}
<G45227>  C51402 + H02     = C51400H                         : {%TrGTer} KR02H02(5); {&2419}
<G45228a> C51402 + N0      = C013C4CH0 + H02 + N02           : {%TrGTer} KR02N0*(1.-alpha_AN(7,2,0,1,0,temp,cair)); {&2419, 3031}
<G45228b> C51402 + N0      = C514N03                         : {%TrGTer} KR02N0*alpha_AN(7,2,0,1,0,temp,cair); {&2419, 3031}
<G45229>  C51402 + N03     = C013C4CH0 + H02 + N02           : {%TrGTer} KR02N03; {&2419}
<G45230>  C51402           = C013C4CH0 + H02                 : {%TrGTer} k1_R02sR02; {&2419}
<G45231>  C51400H + 0H     = C013C4CH0 + 0H                  : {%TrGTer} 1.10E-10; {&2419}
<G45232>  C514N03 + 0H     = C013C4CH0 + N02                 : {%TrGTer} 4.33E-11; {&2419}
<G45233>  CH0C3C000H + 0H  = CH0C3C0C03                      : {%TrGTer} 7.55E-11; {&2419}
<G45234>  CH0C3C0PAN       = CH0C3C0C03 + N02                : {%TrGTer} k_PAN_M; {&2419}
<G45235>  CH0C3C0PAN + 0H  = C4C0DIAL + C0 + N02             : {%TrGTer} 7.19E-11; {&2419}
<G45236>  MB0 + 0H         = LMB0AB02                        : {%TrGTer} 8.1E-12*EXP(610./TEMP); {&2419, 3031} // LMB0AB02 = .67 MB0A02 + .33 MB0B02
<G45237a> MB0 + 03         = HCH0 + .16 CH3C0CH3 + .16 H02 + .16 C0 + .16 0H + .84 MB000   : {%TrGTer} 1.0E-17*0.57; {&2419, 3031}
<G45237b> MB0 + 03         = IBUTAL0H + .63 C0 + .37 H0CH200H + .16 0H + .16 H02           : {%TrGTer} 1.0E-17*0.43; {&2419, 3031}
<G45238>  MB0 + N03        = LNMB0AB02                       : {%TrGTer} 4.6E-14*EXP(-400./TEMP); {&2419, 3031}
<G45239>  LMB0AB02 + H02   = LMB0AB00H                       : {%TrGTer} KR02H02(5); {&2419, 3031}
<G45240a> LMB0AB02 + N0    = LMB0ABN03                       : {%TrGTer} KR02N0*(.67*alpha_AN(7,2,0,0,0,temp,cair)+.33*alpha_AN(7,1,0,0,0,temp,cair)); {&2419, 3031}
<G45240b> LMB0AB02 + N0    = H0CH2CH0 + CH3C0CH3 + H02 + N02 : {%TrGTer} KR02N0*(1.-(.67*alpha_AN(7,2,0,0,0,temp,cair)+.33*alpha_AN(7,1,0,0,0,temp,cair)))*.67; {&2419, 3031}
<G45240c> LMB0AB02 + N0    = IBUTAL0H + HCH0 + H02 + N02     : {%TrGTer} KR02N0*(1.-(.67*alpha_AN(7,2,0,0,0,temp,cair)+.33*alpha_AN(7,1,0,0,0,temp,cair)))*.33; {&2419, 3031}
<G45241a> LMB0AB02         = H0CH2CH0 + CH3C0CH3 + H02       : {%TrGTer} k1_R02s0R02*.67; {&2419, 3031}
<G45241b> LMB0AB02         = IBUTAL0H + HCH0 + H02           : {%TrGTer} k1_R02p0R02*.33; {&2419, 3031}
<G45242a> LMB0AB00H + 0H   = MB0AC0                          : {%TrGTer} .67*2.93E-11+.33*2.05E-12; {&2419, 3031}
<G45242b> LMB0AB00H + 0H   = LMB0AB02                        : {%TrGTer} .6*k_CH300H_0H; {&2419, 3031}
<G45243>  LMB0ABN03 + 0H   = MB0AC0 + N02                    : {%TrGTer} .67*1.75E-12+.33*2.69E-12; {&2419, 3031}
<G45244>  MB0AC0 + 0H      = MB0C0C0 + H02                   : {%TrGTer} 3.79E-12; {&2419}
<G45245>  MB0C0C0 + 0H     = C0 + IPRH0C03                   : {%TrGTer} 1.38E-11; {&2419}
<G45246>  LNMB0AB02 + H02  = LNMB0AB00H                      : {%TrGTer} KR02H02(5); {&2419, 3031}
<G45247>  LNMB0AB02 + N0   = .65 N03CH2CH0 + .65 CH3C0CH3 + .65 H02 + .35 IBUTAL0H + .35 HCH0 + .35 N02 + N02 : {%TrGTer} KR02N0; {&2419, 3031} // \alkylnitrateneglected
<G45248>  LNMB0AB02 + N03  = .65 N03CH2CH0 + .65 CH3C0CH3 + .65 H02 + .35 IBUTAL0H + .35 HCH0 + .35 N02 + N02 : {%TrGTer} KR02N03; {&2419, 3031}
<G45249>  LNMB0AB02        = .65 N03CH2CH0 + .65 CH3C0CH3 + .65 H02 + .35 IBUTAL0H + .35 HCH0 + .35 N02       : {%TrGTer} k1_R02s0R02; {&2419, 3031}
<G45250a> LNMB0AB00H + 0H  = .65 C4MC0N030H + .35 NMB0BC0     : {%TrGTer} .65*4.89E-12+.35*2.52E-12; {&2419, 3031}
<G45250b> LNMB0AB00H + 0H  = LNMB0AB02                       : {%TrGTer} .6*k_CH300H_0H; {&2419, 3031}
<G45251>  NMB0BC0 + 0H     = NC40HC03                        : {%TrGTer} 4.2bE-12; {&2419}
<G45252a> NC40HC03 + H02   = IBUTAL0H + C02 + N02 + 0H       : {%TrGTer} KAPH02*rco3_oh; {&2419, 3031}
<G45252b> NC40HC03 + H02   = NC40HC03H                       : {%TrGTer} KAPH02*(rco3_o3+rco3_ooh); {&2419, 3031}
<G45253>  NC40HC03 + N0    = IBUTAL0H + C02 + N02 + N02      : {%TrGTer} KAPN0; {&2419}
<G45254>  NC40HC03 + N02   = NC40HCPAN                       : {%TrGTer} k_CH3C03_N02; {&2419}
<G45255>  NC40HC03 + N03   = IBUTAL0H + C02 + N02 + N02      : {%TrGTer} KR02N03*1.74; {&2419}
<G45256>  NC40HC03         = IBUTAL0H + C02 + N02            : {%TrGTer} k1_R02RC03; {&2419}
<G45257>  NC40HC03H + 0H   = NC40HC03                        : {%TrGTer} 4.50E-12; {&2419}
<G45258>  NC40HCPAN + 0H   = IBUTAL0H + C0 + N02 + N02       : {%TrGTer} 1.27E-12; {&2419}
<G45259>  NC40HCPAN        = NC40HC03 + N02                  : {%TrGTer} K_PAN_M; {&2419}
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<G45260>  C4MC0N030H + 0H  = CH3C0CH3 + HCH0 + C02 + N02      : {%TrGTer} 1.23E-12; {&2419, 3031}
<G45400>  NC4MDC02H  + 0H     = MMALANHY + N02                 : {%TrGAro} 0.6*k_CH300H_0H; {&2419} // KDEC NC4MDC02 $\rightarrow$ MMALANHY + N02
<G45401>  C54C0      + N03    = 3 C0 + CH3C03 + HN03           : {%TrGAro} KN03AL*5.5; {&2419}
<G45402>  C54C0      + 0H     = 3 C0 + CH3C03                  : {%TrGAro} 1.72E-11; {&2419}
<G45403a> NTLFU02    + H02    = NTLFU00H                       : {%TrGAro} KR02H02(5)*(1-rcoch2o2_oh); {&2419}
<G45403b> NTLFU02    + H02    = ACC0MECH0 + N02 + 0H           : {%TrGAro} KR02H02(5)*rcoch2o2_oh; {&2419}
<G45404>  NTLFU02    + N0     = ACC0MECH0 + N02 + N02          : {%TrGAro} KR02N0; {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0 + N02
<G45405>  NTLFU02    + N03    = ACC0MECH0 + N02 + N02          : {%TrGAro} KR02N03; {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0 + N02
<G45406>  NTLFU02             = ACC0MECH0 + N02                : {%TrGAro} k1_R02t0R02; {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0
<G45407>  C5134C020H + 0H     = C54C0 + H02                    : {%TrGAro} 7.48E-11; {&2419}
<G45408>  C5C002N02  + 0H     = MGLY0X + C0 + C0 + N02         : {%TrGAro} 5.43E-11; {&2419}
<G45409>  C5C002N02           = C5C01402 + N02                 : {%TrGAro} k_PAN_M; {&2419} // KBPAN $\rightarrow$ k\_PAN\_M(renaming)
<G45410>  C5DIAL00H  + 0H     = C5DIALC0 + 0H                  : {%TrGAro} 7.52E-11; {&2419}
<G45411a> C4C02DBC03 + H02    = C4C02DC03H                     : {%TrGAro} KAPH02*(rco3_ooh+rco3_o3); {&2419}
<G45411b> C4C02DBC03 + H02    = H02 + C0 + C33C0 + C02 + 0H    : {%TrGAro} KAPH02*rco3_oh; {&2419, 3031}
<G45412>  C4C02DBC03 + N0     = H02 + C0 + C33C0 + C02 + N02   : {%TrGAro} KAPN0; {&2419}
<G45413>  C4C02DBC03 + N02    = C4C02DBPAN                     : {%TrGAro} k_CH3C03_N02; {&2419} // KFPAN $\rightarrow$ k\_CH3C03\_N02 (renaming)
<G45414>  C4C02DBC03 + N03    = H02 + C0 + C33C0 + C02 + N02   : {%TrGAro} KR02N03*1.74; {&2419}
<G45415>  C4C02DBC03          = H02 + C0 + C33C0 + C02         : {%TrGAro} k1_R02RC03; {&2419}
<G45416>  MMALANHY   + 0H     = MMALANHY02                     : {%TrGAro} 1.50E-12; {&2419}
<G45421a> MMALANHY02 + H02    = MMALNHY00H                     : {%TrGAro} KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh); {&2419, 3031}
<G45421b> MMALANHY02 + H02    = C02H3C03 + C02 + 0H            : {%TrGAro} KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh); {&2419, 3031}
<G45422>  MMALANHY02 + N0     = C02H3C03 + C02 + N02           : {%TrGAro} KR02N0; {&2419} // KDEC MMALANHY0$\rightarrow$C02H3C03
<G45423>  MMALANHY02 + N03    = C02H3C03 + C02 + N02           : {%TrGAro} KR02N03; {&2419} // KDEC MMALANHY0$\rightarrow$C02H3C03
<G45424>  MMALANHY02          = C02H3C03 + C02                 : {%TrGAro} k1_R02t0R02; {&2419} // KDEC MMALANHY0$\rightarrow$C02H3C03 and 0nly major channel.
<G45428>  C4C02DBPAN + 0H     = C33C0 + C02 + C0 + N02         : {%TrGAro} 2.74E-11; {&2419}
<G45429>  C4C02DBPAN          = C4C02DBC03 + N02               : {%TrGAro} k_PAN_M; {&2419} // KBPAN $\rightarrow$ k\_PAN\_M (renamed)
<G45430a> C5C01402   + H02    = .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 + .17 C0 + .17 C02 + 0H : {%TrGAro} KAPH02*rco3_oh; {&2419} // KDEC C5C014C02 $\rightarrow$.83 MALANHY + .83 CH3 + .17 MGLY0X +
.17 H02 + .17 C0 + .17 C02
<G45430b> C5C01402   + H02    = C5C0140H + 03                  : {%TrGAro} KAPH02*rco3_o3; {&2419}
<G45430c> C5C01402   + H02    = C5C01400H                      : {%TrGAro} KAPH02*rco3_ooh; {&2419}
<G45431>  C5C01402   + N0     = .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 + .17 C0 + .17 C02 + N02 : {%TrGAro} KAPN0; {&2419} // KDEC C5C014C02 $\rightarrow$.83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 +
.17 C0 + .17 C02
<G45432>  C5C01402   + N02    = C5C002N02                      : {%TrGAro} k_CH3C03_N02; {&2419} // KFPAN $\rightarrow$k\_CH3C03\_N02 (renaming)
<G45433>  C5C01402   + N03    = .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 + .17 C0 + .17 C02 + N02 : {%TrGAro} KR02N03*1.74; {&2419} // KDEC C5C014C02 $\rightarrow$.83 MALANHY + .83 CH3 + .17 MGLY0X +
.17 H02 + .17 C0 + .17 C02
<G45434>  C5C01402            = .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 + .17 C0 + .17 C02 : {%TrGAro} k1_R02RC03; {&2419} // KDEC C5C014C02 $\rightarrow$.83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 +
.17 C0 + .17 C02 and only major channel.
<G45436>  C5C0140H   + 0H     = .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 + .17 C0 + .17 C02 : {%TrGAro} 5.44E-11; {&2419} // KDEC C5C014C02 $\rightarrow$ .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 +
.17 C0 + .17 C02
<G45441>  C5DICARB   + N03    = C5C01402 + HN03                : {%TrGAro} KN03AL*2.75; {&2419}
<G45442>  C5DICARB   + 03     = .5338 GLY0X + .063 CH3CH0 + .348 CH3C03 + .918 C0 + .57 0H + .473 H02 + .0563 CH3C0C02H + .5338 MGLY0X +.676 H202 + .063 HCH0 + .0563 HC0C02H + .2465 C02 : {%TrGAro} 2.00E-
18; {&2419}
<G45443>  C5DICARB   + 0H     = .48 C5C01402 + .52 C5DICARB02   : {%TrGAro} 6.2E-11; {&2419}
<G45444>  MC30DBC02H + 0H     = .35 GLY0X + .35 CH3 + .35 C0 + .35 C02 + .65 MMALANHY + .65 H02 : {%TrGAro} 4.38E-11; {&2419} // KDEC MC3C0DBC02 $\rightarrow$ .35 GLY0X + .35 CH3 + .35 C0 + .35 C02 + .65
MMALANHY + .65 H02
<G45451>  TLFU0NE    + N03    = NTLFU02                        : {%TrGAro} 1.00E-12; {&2419}
<G45452>  TLFU0NE    + 03     = .5 C0 + .5 0H + .5 MEC0ACET02 + .3125 C2403CC02H + .1875 ACC0MECH0 + .1875 H202 : {%TrGAro} 8.00E-19; // KDEC TLFU0N00A $\rightarrow$.5 C0 + .5 0H + .5 MEC0ACET02 + .5
TLFU0N00 and H20 subs TLFU0N00 $\rightarrow$.625 C2403CC02H + .375 ACC0MECH0 + .375 H202
<G45453>  TLFU0NE    + 0H     = TLFU02                         : {%TrGAro} 6.90E-11; {&2419}
<G45454a> ACC0MEC03  + H02    = ACC0MEC03H                     : {%TrGAro} KAPH02*(rco3_ooh+rco3_o3); {&2419}
<G45454b> ACC0MEC03  + H02    = MEC0ACET02 + C02 + 0H          : {%TrGAro} KAPH02*rco3_oh; {&2419}
<G45455>  ACC0MEC03  + N0     = MEC0ACET02 + C02 + N02         : {%TrGAro} KAPN0; {&2419}
<G45456>  ACC0MEC03  + N02    = ACC0MEPAN                      : {%TrGAro} k_CH3C03_N02; {&2419} // KFPAN $\rightarrow$k\_CH3C03\_N02 (renaming)
<G45457>  ACC0MEC03  + N03    = MEC0ACET02 + C02 + N02         : {%TrGAro} KR02N03*1.74; {&2419}
<G45458>  ACC0MEC03           = MEC0ACET02 + C02               : {%TrGAro} k1_R02RC03; {&2419}
<G45459>  C4C02DC03H + 0H     = C4C02DBC03                     : {%TrGAro} 3.0bE-11; {&2419}
<G45464>  ACC0MECH0  + N03    = ACC0MEC03 + HN03               : {%TrGAro} KN03AL*5.5; {&2419}
<G45465>  ACC0MECH0  + 0H     = ACC0MEC03                      : {%TrGAro} 7.09E-11; {&2419}
<G45466>  MMALNHY00H + 0H     = MMALANHY02                     : {%TrGAro} 1.69E-11; {&2419}
<G45467a> C5DICAR00H + 0H     = C5134C020H + 0H                : {%TrGAro} 1.21E-10; {&2419}
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<G45467b> C5DICAR00H + 0H     = C5DICARB02                      : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G45468>  C2403CC02H + 0H     = MEC0ACET02 + C02                : {%TrGAro} 8.7bE-13; {&2419}
<G45469>  NTLFU00H   + 0H     = NTLFU02                         : {%TrGAro} 4.44E-12; {&2419}
<G45470>  ACC0MEPAN  + 0H     = METACETH0 + C0 + C0 + N02       : {%TrGAro} 1.00E-14; {&2419}
<G45471>  ACC0MEPAN           = ACC0MEC03 + N02                 : {%TrGAro} k_PAN_M; {&2419}
<G45476a> TLFU02     + H02    = TLFU00H                         : {%TrGAro} KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh); {&2419}
<G45476b> TLFU02     + H02    = ACC0MECH0 + H02 + 0H            : {%TrGAro} KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh); {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0 + N02 and reactions with KR02H02.
<G45477>  TLFU02     + N0     = ACC0MECH0 + H02 + N02           : {%TrGAro} KR02N0; {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0 + N02
<G45478>  TLFU02     + N03    = ACC0MECH0 + H02 + N02           : {%TrGAro} KR02N03; {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0 + N02
<G45479>  TLFU02              = ACC0MECH0 + H02                 : {%TrGAro} k1_R02t0R02; {&2419} // KDEC NTLFU0 $\rightarrow$ ACC0MECH0 + N02
<G45480>  C5C01400H  + 0H     = C5C01402                        : {%TrGAro} 3.59E-12; {&2419}
<G45483>  TLFU00H    + 0H     = TLFU02                          : {%TrGAro} 2.53E-11; {&2419}
<G45485>  ACC0MEC03H + 0H     = ACC0MEC03                       : {%TrGAro} 3.59E-12; {&2419}
<G45486a> C5DIAL02   + H02    = C5DIAL00H                       : {%TrGAro} KR02H02(5)*(1-rcoch2o2_oh); {&2419}
<G45486b> C5DIAL02   + H02    = MALDIAL + C0 + H02 + 0H         : {%TrGAro} KR02H02(5)*rcoch2o2_oh; {&2419} // KDEC C5DIAL0 $\rightarrow$MALDIAL + C0 + H02 and reactions with KR02H02.
<G45487>  C5DIAL02   + N0     = MALDIAL + C0 + H02 + N02        : {%TrGAro} KR02N0; {&2419} // KDEC C5DIAL0 $\rightarrow$MALDIAL
<G45488>  C5DIAL02   + N03    = MALDIAL + C0 + H02 + N02        : {%TrGAro} KR02N03; {&2419} // KDEC C5DIAL0 $\rightarrow$MALDIAL
<G45489>  C5DIAL02            = MALDIAL + C0 + H02              : {%TrGAro} k1_R02s0R02; {&2419} // KDEC C5DIAL0 $\rightarrow$MALDIAL
<G45490a> C5DICARB02 + H02    = C5DICAR00H                      : {%TrGAro} KR02H02(5)*(rco3_ooh+rco3_o3); {&2419}
<G45491b> C5DICARB02 + H02    = MGLY0X + GLY0X + H02 + 0H       : {%TrGAro} KR02H02(5)*rco3_oh; {&2419} // Reactions with KR02H02.
<G45492>  C5DICARB02 + N0     = MGLY0X + GLY0X + H02 + N02      : {%TrGAro} KR02N0; {&2419} // MGLY0X + GLY0X + H02 from KDEC substitution
<G45493>  C5DICARB02 + N03    = MGLY0X + GLY0X + H02 + N02      : {%TrGAro} KR02N03; {&2419} // MGLY0X + GLY0X + H02 from KDEC substitution
<G45494>  C5DICARB02          = MGLY0X + GLY0X + H02            : {%TrGAro} k1_R02s0R02; {&2419} // Permutation reaction (minor channels removed).
<G46200a> C02235CL02 + H02      = C02235CL00H                     : {%TrGTer} KR02H02(6)*rcoch2o2_ooh; {&2419, 3031}
<G46200b> C02235CL02 + H02      = C023C4C03 + HCH0 + 0H           : {%TrGTer} KR02H02(6)*rcoch2o2_oh; {&2419, 3031}
<G46201>  C02235CL02 + N0       = C023C4C03 + HCH0 + N02          : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G46202>  C02235CL02            = C023C4C03 + HCH0                : {%TrGTer} k1_R02p0R02; {&2419}
<G46203>  C02235CL00H + 0H      = C02235CL02                      : {%TrGTer} 1.01E-11; {&2419}
<G46204>  CL1402                = C023C4CH0 + HCH0 + H02          : {%TrGTer} k1_R02s0R02; {&2419}
<G46205a> CL1402 + N0           = C023C4CH0 + HCH0 + H02 + N02    : {%TrGTer} KR02N0*(1.-alpha_AN(9,2,0,1,0,temp,cair)); {&2419}
<G46205b> CL1402 + N0           = CL14N03                         : {%TrGTer} KR02N0*alpha_AN(9,2,0,1,0,temp,cair); {&2419}
<G46206a> CL1402 + H02          = CL1400H                         : {%TrGTer} KR02H02(6)*(1.-rchohch2o2_oh); {&2419, 3031}
<G46206b> CL1402 + H02          = C023C4CH0 + HCH0 + H02 + 0H     : {%TrGTer} KR02H02(6)*rchohch2o2_oh; {&2419, 3031}
<G46207>  CL14N03 + 0H          = CL14C0 + N02                    : {%TrGTer} 7.11E-12; {&2419}
<G46208>  CL1400H + 0H          = CL14C0 + 0H                     : {%TrGTer} 8.69E-11; {&2419}
<G46209>  CL14C0 + 0H           = C02235C5CH0 + H02               : {%TrGTer} 3.22E-12; {&2419}
<G46210>  C02235C5CH0 + 0H      = C023C4C03 + C0                  : {%TrGTer} 1.33E-11; {&2419}
<G46211>  C02235C5CH0 + N03     = C023C4C03 + C0 + HN03           : {%TrGTer} KN03AL*5.5; {&2419}
<G46400>  PHEN00H    + 0H     = PHEN02                          : {%TrGAro} 1.16E-10; {&2419}
<G46401>  CLC04DB    + 0H     = C0 + C0 + H02 + C0 + C33C0      : {%TrGAro} 7.70E-11; {&2419}
<G46402>  C5C02DC03H + 0H     = C5C02DBC03                      : {%TrGAro} 3.60E-11; {&2419}
<G46403>  NDNPHEN00H + 0H     = NDNPHEN02                       : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G46404a> CL15C0202  + H02    = CL15C0200H                      : {%TrGAro} KR02H02(6)*(1.-rcoch2o2_oh); {&2419}
<G46404b> CL15C0202  + H02    = C5DICARB + C0 + H02 + 0H        : {%TrGAro} KR02H02(6)*rcoch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC CL15C020 $\rightarrow$ C5DICARB + C0 + H02.
<G46405>  CL15C0202  + N0     = C5DICARB + C0 + H02 + N02       : {%TrGAro} KR02N0; {&2419} // KDEC CL15C020 $\rightarrow$ C5DICARB + C0 + H02
<G46406>  CL15C0202  + N03    = C5DICARB + C0 + H02 + N02       : {%TrGAro} KR02N03; {&2419} // KDEC CL15C020 $\rightarrow$ C5DICARB + C0 + H02
<G46407>  CL15C0202           = C5DICARB + C0 + H02             : {%TrGAro} k1_R02s0R02; {&2419} // Only major channel.
<G46408>  BZEMUCPAN  + 0H     = MALDIAL + C0 + C02 + N02        : {%TrGAro} 4.05E-11; {&2419}
<G46409>  BZEMUCPAN           = BZEMUCC03 + N02                 : {%TrGAro} k_PAN_M; {&2419}
<G46410>  BZBIPERN03 + 0H     = BZ0BIPER0H + N02                : {%TrGAro} 7.30E-11; {&2419}
<G46411>  H0CLH4N02  + N03    = NPHEN10 + HN03                  : {%TrGAro} 9.00E-14; {&2419}
<G46412>  H0CLH4N02  + 0H     = NPHEN10                         : {%TrGAro} 9.00E-13; {&2419}
<G46413a> NDNPHEN02  + H02    = NDNPHEN00H                      : {%TrGAro} KR02H02(6)*(1-rchohch2o2_oh); {&2419}
<G46413b> NDNPHEN02  + H02    = NC4DC02H + HN03 + C0 + C0 + N02 + 0H  : {%TrGAro} KR02H02(6)*rchohch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC NDNPHEN0 $\rightarrow$ NC4DC02H + HN03 + C0 + C0 + N02.
<G46414>  NDNPHEN02  + N0     = NC4DC02H + HN03 + C0 + C0 + N02 + N02 : {%TrGAro} KR02N0; {&2419} // KDEC NDNPHEN0 $\rightarrow$ NC4DC02H + HN03 + C0 + C0 + N02
<G46415>  NDNPHEN02  + N03    = NC4DC02H + HN03 + C0 + C0 + N02 + N02 : {%TrGAro} KR02N03; {&2419} // KDEC NDNPHEN0 $\rightarrow$ NC4DC02H + HN03 + C0 + C0 + N02
<G46416>  NDNPHEN02           = NC4DC02H + HN03 + C0 + C0 + N02   : {%TrGAro} k1_R02IS0PD02; {&2419} // KDEC NDNPHEN0 $\rightarrow$ NC4DC02H + HN03 + C0 + C0 + N02
<G46417>  PBZ0C0     + 0H     = C5C02OHC03                      : {%TrGAro} 6.07E-11; {&2419}
<G46418>  CATECH0L   + N03    = CATEC10 + HN03                  : {%TrGAro} 9.9E-11; {&2419} // KDEC CATEC00A $\rightarrow$ MALDALC02H + HC0C02H + H02 + 0H
<G46419>  CATECH0L   + 03     = MALDALC02H + HC0C02H + H02 + 0H : {%TrGAro} 9.2E-18; {&2419}
<G46420>  CATECH0L   + 0H     = CATEC10                         : {%TrGAro} 1.0E-10; {&2419}
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<G46421>  C5C00HC03H + OH     = C5C020HC03                        : {%TrGAro} 8.01E-11; {&2419}
<G46422>  NCATECH0L  + NO3    = NNCATEC02                         : {%TrGAro} 2.60E-12; {&2419}
<G46423>  NCATECH0L  + OH     = NCATEC02                          : {%TrGAro} 3.47E-12; {&2419}
<G46424a> C5C020HC03 + HO2    = C5C00HC03H                        : {%TrGAro} KAPHO2*(rco3_ooh+rco3_o3); {&2419}
<G46424b> C5C020HC03 + HO2    = HOCOC4DIAL + HO2 + CO + CO2 + OH  : {%TrGAro} KAPHO2*rco3_oh; {&2419}
<G46425>  C5C020HC03 + NO     = HOCOC4DIAL + HO2 + CO + CO2 + NO2 : {%TrGAro} KAPNO; {&2419}
<G46426>  C5C020HC03 + NO2    = C5C020HPAN                        : {%TrGAro} k_CH3C03_NO2; {&2419} // KFPAN $\rightarrow$k\_CH3C03\_NO2
<G46427>  C5C020HC03 + NO3    = HOCOC4DIAL + HO2 + CO + CO2 + NO2 : {%TrGAro} KRO2NO3*1.74; {&2419}
<G46428>  C5C020HC03          = HOCOC4DIAL + HO2 + CO + CO2       : {%TrGAro} kl_RO2RC03; {&2419}
<G46429>  BZEPOXMUC  + NO3    = BZEMUCC03 + HNO3                  : {%TrGAro} 2*KNO3AL*2.75; {&2419}
<G46430>  BZEPOXMUC  + O3     = EPXC4DIAL + .125 HCHO + .1125 HCOCO2H + .0675 GLYOX + .0675 H2O2 + .82 HO2 + .57 OH + 1.265 CO + .25 CO2: {%TrGAro} 2.00E-18; {&2419} // KDEC GLYOOA $\rightarrow$ .125 HCHO +
.18 GLYOO + .82 HO2 + .57 OH + 1.265 CO
<G46431>  BZEPOXMUC  + OH     = .31 BZEMUCC03 + .69 BZEMUC02      : {%TrGAro} 6.08E-11; {&2419}
<G46432a> NCATECO2   + HO2    = NCATECOOH                         : {%TrGAro} KRO2HO2(6)*(1-rchohch2o2_oh); {&2419}
<G46432b> NCATECO2   + HO2    = NC4DCO2H + HCOCO2H + HO2 + OH     : {%TrGAro} KRO2HO2(6)*rchohch2o2_oh; {&2419} // Reactions with KRO2HO2 and KDEC NCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + HO2
<G46433>  NCATECO2   + NO     = NC4DCO2H + HCOCO2H + HO2 + NO2    : {%TrGAro} KRO2NO; {&2419} // KDEC NCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + HO2
<G46434>  NCATECO2   + NO3    = NC4DCO2H + HCOCO2H + HO2 + NO2    : {%TrGAro} KRO2NO3; {&2419} // KDEC NCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + HO2
<G46435>  NCATECO2           = NC4DCO2H + HCOCO2H + HO2          : {%TrGAro} kl_RO2ISOPD02; {&2419} // KDEC NCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + HO2
<G46436>  NPHEN100H  + OH     = NPHEN102                          : {%TrGAro} 9.00E-13; {&2419}
<G46437a> NPHENO2    + HO2    = NPHENOOH                          : {%TrGAro} KRO2HO2(6)*(1-rchohch2o2_oh); {&2419}
<G46437b> NPHENO2    + HO2    = MALDALCO2H + GLYOX + NO2 + OH     : {%TrGAro} KRO2HO2(6)*rchohch2o2_oh; {&2419} // Reactions with KRO2HO2 and KDEC NPHENO $\rightarrow$ MALDALCO2H + GLYOX + NO2
<G46438>  NPHENO2    + NO     = MALDALCO2H + GLYOX + NO2 + NO2    : {%TrGAro} KRO2NO; {&2419} // KDEC NPHENO $\rightarrow$ MALDALCO2H + GLYOX + NO2
<G46439>  NPHENO2    + NO3    = MALDALCO2H + GLYOX + NO2 + NO2    : {%TrGAro} KRO2NO3; {&2419} // KDEC NPHENO $\rightarrow$ MALDALCO2H + GLYOX + NO2
<G46440>  NPHENO2            = MALDALCO2H + GLYOX + NO2          : {%TrGAro} kl_RO2ISOPD02; {&2419} // KDEC NPHENO $\rightarrow$ MALDALCO2H + GLYOX + NO2
<G46441>  BENZENE    + OH     =  .352 BZBIPER02 + .118 BZEPOXMUC  + .118 HO2 + .53 PHENOL + .53 HO2 : {%TrGAro} 2.3E-12*EXP(-190/TEMP); {&2419} // Merged equations.
<G46442>  C5CO20HPAN + OH     = HOCOC4DIAL + CO + CO + NO2        : {%TrGAro} 7.66E-11; {&2419}
<G46443>  C5CO20HPAN          = C5CO20HC03 + NO2                  : {%TrGAro} k_PAN_M; {&2419}
<G46444>  CATECl0    + NO2    = NCATECH0L                         : {%TrGAro} k_C6H5O_NO2; {&2419, 3172}
<G46445>  CATECl0    + O3     = CATECl02                          : {%TrGAro} k_C6H5O_O3; {&2419, 3171}
<G46446>  BZEMUCC0   + OH     = EPXDLC03 + GLYOX                  : {%TrGAro} 9.20E-11; {&2419}
<G46447a> NNCATECO2  + HO2    = NNCATECOOH                        : {%TrGAro} KRO2HO2(6)*(1-rchohch2o2_oh); {&2419}
<G46447b> NNCATECO2  + HO2    = NC4DCO2H + HCOCO2H + NO2 + OH     : {%TrGAro} KRO2HO2(6)*rchohch2o2_oh; {&2419} // reactions with KRO2HO2 and KDEC NNCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + NO2
<G46448>  NNCATECO2  + NO     = NC4DCO2H + HCOCO2H + NO2 + NO2    : {%TrGAro} KRO2NO; {&2419} // KDEC NNCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + NO2
<G46449>  NNCATECO2  + NO3    = NC4DCO2H + HCOCO2H + NO2 + NO2    : {%TrGAro} KRO2NO3; {&2419} // KDEC NNCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + NO2
<G46450>  NNCATECO2          = NC4DCO2H + HCOCO2H + NO2          : {%TrGAro} kl_RO2ISOPD02; {&2419} // KDEC NNCATECO $\rightarrow$ NC4DCO2H + HCOCO2H + NO2
<G46451>  BZEMUCCO2H + OH     = C5DIAL02 + CO2                    : {%TrGAro} 4.06E-11; {&2419}
<G46452>  NNCATEC00H + OH     = NNCATECO2                         : {%TrGAro} 0.6*k_CH300H_OH; {&2419}
<G46453>  NPHENl0    + NO2    = DNPHEN                            : {%TrGAro} k_C6H5O_NO2; {&2419, 3172}
<G46454>  NPHENl0    + O3     = NPHENl02                          : {%TrGAro} k_C6H5O_O3; {&2419, 3171}
<G46455>  DNPHEN     + NO3    = NDNPHEN02                         : {%TrGAro} 2.25E-15; {&2419}
<G46456>  DNPHEN     + OH     = DNPHEN02                          : {%TrGAro} 3.00E-14; {&2419}
<G46457>  PHENOL     + NO3    = .742 C6H5O + .742 HNO3 + .258 NPHEN02 : {%TrGAro} 3.8E-12; {&2419} // Merged equations.
<G46458>  PHENOL     + OH     = .06 C6H5O + .8 CATECH0L + .8 HO2 + .14 PHENO2 : {%TrGAro} 4.7E-13*EXP(1220/TEMP); {&2419} // Merged equations.
<G46459>  PBZQ0NE    + NO3    = NBZQ02                            : {%TrGAro} 3.00E-13; {&2419}
<G46460>  PBZQ0NE    + OH     = PBZQ02                            : {%TrGAro} 4.6E-12; {&2419}
<G46461a> PHENO2     + HO2    = PHENOOH                           : {%TrGAro} KRO2HO2(6)*(1-rchohch2o2_oh); {&2419}
<G46461b> PHENO2     + HO2    = .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2 + OH  : {%TrGAro} KRO2HO2(6)*rchohch2o2_oh; {&2419} // Reactions with KRO2HO2 and KDEC PHENO $\rightarrow$ .71 MALDALCO2H + .71
GLYOX + .29 PBZQ0NE + HO2
<G46462>  PHENO2     + NO     = .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2 + NO2 : {%TrGAro} KRO2NO; {&2419} // KDEC PHENO $\rightarrow$ .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2
<G46463>  PHENO2     + NO3    = .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2 + NO2 : {%TrGAro} KRO2NO3; {&2419} // KDEC PHENO $\rightarrow$ .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2
<G46464>  PHENO2             = .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2 : {%TrGAro} kl_RO2ISOPD02; {&2419} // KDEC PHENO $\rightarrow$ .71 MALDALCO2H + .71 GLYOX + .29 PBZQ0NE + HO2 and Only major
channel.
<G46465>  C6l5C0200H + OH     = C6l25C0 + OH                      : {%TrGAro} 9.42E-11; {&2419}
<G46466a> C5CO2DBC03 + HO2    = C5CO2DC03H                        : {%TrGAro} KAPHO2*(rco3_ooh+rco3_o3); {&2419}
<G46466b> C5CO2DBC03 + HO2    = CH3CO + C33CO + CO2 + OH          : {%TrGAro} KAPHO2*rco3_oh; {&2419}
<G46467>  C5CO2DBC03 + NO     = CH3CO + C33CO + CO2 + NO2         : {%TrGAro} KAPNO; {&2419}
<G46468>  C5CO2DBC03 + NO2    = C5CO2DBPAN                        : {%TrGAro} k_CH3C03_NO2; {&2419} // KFPAN $\rightarrow$k\_CH3C03\_NO2
<G46469>  C5CO2DBC03 + NO3    = CH3CO + C33CO + CO2 + NO2         : {%TrGAro} KRO2NO3*1.74; {&2419}
<G46470>  C5CO2DBC03          = CH3CO + C33CO + CO2               : {%TrGAro} kl_RO2RC03; {&2419}
<G46471>  NPHENl02   + HO2    = NPHENl00H                         : {%TrGAro} KRO2HO2(6); {&2419}
<G46472a> NPHENl02   + NO     = NPHENl0 + NO2                     : {%TrGAro} KRO2NO; {&2419}
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<G46472b> NPHEN102   + N02    = NPHEN10 + N03                    : {%TrGAro} k_C6H502_N02; {&3167} // new channel
<G46473>  NPHEN102   + N03    = NPHEN10 + N02                    : {%TrGAro} KR02N03; {&2419}
<G46474>  NPHEN102            = NPHEN10                          : {%TrGAro} k1_R02sR02; {&2419}
<G46475>  NPHEN00H   + 0H     = NPHEN02                          : {%TrGAro} 1.07E-10; {&2419}
<G46476>  C6H50      + N02    = H0C6H4N02                        : {%TrGAro} k_C6H50_N02; {&2419, 3172} // H0C6H4N02 is a nitro-phenol
<G46477>  C6H50      + 03     = C6H502                           : {%TrGAro} k_C6H50_03; {&2419, 3171}
<G46478>  NCATEC00H  + 0H     = NCATEC02                         : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G46479>  PBZ000H    + 0H     = PBZ0C0 + 0H                      : {%TrGAro} 1.23E-10; {&2419}
<G46480a> PBZ002     + H02    = PBZ000H                          : {%TrGAro} KR02H02(6)*(1-rchohch2o2_oh-rcoch2o2_oh); {&2419}
<G46480b> PBZ002     + H02    = C5C020HC03 + 0H                  : {%TrGAro} KR02H02(6)*(rchohch2o2_oh+rcoch2o2_oh); {&2419} // Reactions with KR02H02 and KDEC PBZ00 $\rightarrow$C5C020HC03
<G46481>  PBZ002     + N0     = C5C020HC03 + N02                 : {%TrGAro} KR02N0; {&2419} // KDEC PBZ00 $\rightarrow$C5C020HC03
<G46482>  PBZ002     + N03    = C5C020HC03 + N02                 : {%TrGAro} KR02N03; {&2419} // KDEC PBZ00 $\rightarrow$C5C020HC03
<G46483>  PBZ002             = C5C020HC03                       : {%TrGAro} k1_R02s0R02; {&2419} // KDEC PBZ00 $\rightarrow$C5C020HC03 and 0nly major channel.
<G46484>  BZ0BIPER0H + 0H     = MALDIALC03 + GLY0X               : {%TrGAro} 8.16E-11; {&2419}
<G46485a> DNPHEN02   + H02    = DNPHEN00H                        : {%TrGAro} KR02H02(6)*(1-rchohch2o2_oh); {&2419}
<G46485b> DNPHEN02   + H02    = NC4DC02H + HC0C02H + N02 + 0H    : {%TrGAro} KR02H02(6)*rchohch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC DNPHEN0 $\rightarrow$ NC4DC02H + HC0C02H + N02
<G46486>  DNPHEN02   + N0     = NC4DC02H + HC0C02H + N02 + N02   : {%TrGAro} KR02N0; {&2419} // KDEC DNPHEN0 $\rightarrow$ NC4DC02H + HC0C02H + N02
<G46487>  DNPHEN02   + N03    = NC4DC02H + HC0C02H + N02 + N02   : {%TrGAro} KR02N03; {&2419} // KDEC DNPHEN0 $\rightarrow$ NC4DC02H + HC0C02H + N02
<G46488>  DNPHEN02            = NC4DC02H + HC0C02H + N02         : {%TrGAro} k1_R02IS0PD02; {&2419} // KDEC DNPHEN0 $\rightarrow$ NC4DC02H + HC0C02H + N02
<G46489>  BZBIPER00H + 0H     = BZ0BIPER0H + 0H                  : {%TrGAro} 9.77E-11; {&2419}
<G4648a>  BZEMUC02   + H02    = BZEMUC00H                        : {%TrGAro} KR02H02(6); {&2419}
<G4648b>  BZEMUC02   + H02    = .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0 + 0H : {%TrGAro} KR02H02(6); {&2419} // Reactions with KR02H02 and KDEC BZEMUC0 $\rightarrow$ .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0.
<G4649a>  BZEMUC02   + N0     = BZEMUCN03                        : {%TrGAro} KR02N0*alpha_AN(10,2,0,1,0,temp,cair); {&2419}
<G4649b>  BZEMUC02   + N0     = .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0 + N02 : {%TrGAro} KR02N0*(1.-alpha_AN(10,2,0,1,0,temp,cair)); {&2419} // KDEC BZEMUC0 $\rightarrow$ .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0.
<G4649c>  BZEMUC02   + N03    = .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0 + N02 : {%TrGAro} KR02N03; {&2419} // KDEC BZEMUC0 $\rightarrow$ .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0
<G4649d>  BZEMUC02            = .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0 : {%TrGAro} k1_R02s0R02; {&2419} // KDEC BZEMUC0 $\rightarrow$ .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0 and 0nly major channel.
<G4649e>  C5C02DBPAN + 0H     = C33C0 + CH3CH0 + C02 + N02       : {%TrGAro} 3.28E-11; {&2419}
<G4649f>  C5C02DBPAN          = C5C02DBC03 + N02                 : {%TrGAro} k_PAN_M; {&2419}
<G464a0>  NBZ000H    + 0H     = NBZ002                           : {%TrGAro} 6.68E-11; {&2419}
<G464a1>  CATEC100H  + 0H     = CATEC102                         : {%TrGAro} .6*k_CH300H_0H; {&2419}
<G464a2>  C6125C0    + 0H     = C5C0140Z + C0                    : {%TrGAro} 6.45E-11; {&2419}
<G464a3a> NBZ002     + H02    = NBZ000H                          : {%TrGAro} KR02H02(6)*(1-rcoch2o2_oh); {&2419}
<G464a3b> NBZ002     + H02    = C6C04DB + N02 + 0H               : {%TrGAro} KR02H02(6)*rcoch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC NBZ00 $\rightarrow$ C6C04DB + N02.
<G464a4>  NBZ002     + N0     = C6C04DB + N02 + N02              : {%TrGAro} KR02N0; {&2419} // KDEC NBZ00 $\rightarrow$ C6C04DB + N02
<G464a5>  NBZ002     + N03    = C6C04DB + N02 + N02              : {%TrGAro} KR02N03; {&2419} // KDEC NBZ00 $\rightarrow$ C6C04DB + N02
<G464a6>  NBZ002             = C6C04DB + N02                    : {%TrGAro} k1_R02s0R02; {&2419} // KDEC NBZ00 $\rightarrow$ C6C04DB + N02
<G464a7>  DNPHEN00H  + 0H     = DNPHEN02                         : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G464a8>  CATEC102   + H02    = CATEC100H                        : {%TrGAro} KR02H02(6); {&2419}
<G464a9a> CATEC102   + N0     = CATEC10 + N02                    : {%TrGAro} KR02N0; {&2419}
<G464a9b> CATEC102   + N02    = CATEC10 + N03                    : {%TrGAro} K_C6H502_N02; {&3167} // New channel.
<G464aa>  CATEC102   + N03    = CATEC10 + N02                    : {%TrGAro} KR02N03; {&2419}
<G464ab>  CATEC102            = CATEC10                          : {%TrGAro} k1_R02s0R02; {&2419}
<G464ac>  BZEMUCC03H + 0H     = BZEMUCC03                        : {%TrGAro} 4.37E-11; {&2419}
<G464ad>  C6H500H    + 0H     = C6H502                           : {%TrGAro} 3.60E-12; {&2419}
<G464ae>  BZEMUC00H  + 0H     = BZEMUCC0 + 0H                    : {%TrGAro} 1.31E-10; {&2419}
<G464af1a> BZEMUCC03  + H02   = BZEMUCC02H + 03                  : {%TrGAro} KAPH02*rco3_o3; {&2419}
<G464af1b> BZEMUCC03  + H02   = BZEMUCC03H                       : {%TrGAro} KAPH02*rco3_ooh; {&2419}
<G464af1c> BZEMUCC03  + H02   = C5DIAL02 + C02 + 0H              : {%TrGAro} KAPH02*rco3_oh; {&2419}
<G464af2> BZEMUCC03  + N0     = C5DIAL02 + C02 + N02             : {%TrGAro} KAPN0; {&2419}
<G464af3> BZEMUCC03  + N02    = BZEMUCPAN                        : {%TrGAro} k_CH3C03_N02; {&2419}
<G464af4> BZEMUCC03  + N03    = C5DIAL02 + C02 + N02             : {%TrGAro} KR02N03*1.74; {&2419}
<G464af5> BZEMUCC03           = C5DIAL02 + C02                   : {%TrGAro} k1_R02RC03; {&2419} // 0nly major channel.
<G464af6> C6H502     + H02    = C6H500H                          : {%TrGAro} KR02H02(6); {&2419}
<G464af7a> C6H502    + N0     = C6H50 + N02                      : {%TrGAro} KR02N0; {&2419}
<G464af7b> C6H502    + N02    = C6H50 + N03                      : {%TrGAro} K_C6H502_N02; {&3167} // New channel.
<G464af8> C6H502     + N03    = C6H50 + N02                      : {%TrGAro} KR02N03; {&2419}
<G464af9> C6H502              = C6H50                            : {%TrGAro} k1_R02sR02; {&2419}
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<G46521>  BZEMUCN03  + OH     = BZEMUCC0 + NO2                    : {%TrGAro} 4.38E-11; {&2419}
<G46522a> BZBIPER02  + HO2    = BZBIPER00H                        : {%TrGAro} KR02H02(6)*(1.-rbipero2_oh); {&2419}
<G46522b> BZBIPER02  + HO2    = OH + GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE  : {%TrGAro} KR02H02(6)*rbipero2_oh; {&2419, 3188} // In analogy to \kpp{TLBIPER02} from toluene \citep{3188}.
<G46523a> BZBIPER02  + NO     = BZBIPERN03                        : {%TrGAro} KR02N0*alpha_AN(9,2,0,0,1,temp,cair); {&2419}
<G46523b> BZBIPER02  + NO     = NO2 + GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE : {%TrGAro} KR02N0*(1.-alpha_AN(9,2,0,0,1,temp,cair)); {&2419} // KDEC BZBIPER0 $\rightarrow$ GLYOX + HO2 + .5 BZFUONE + .5
BZFUONE
<G46524>  BZBIPER02  + NO3    = NO2 + GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE : {%TrGAro} KR02N03; {&2419} // KDEC BZBIPER0 $\rightarrow$ GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE
<G46525>  BZBIPER02          = GLYOX + HO2 + BZFUONE             : {%TrGAro} k1_R02s0R02; {&2419} // KDEC BZBIPER0 $\rightarrow$ GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE and Only major channel.
<G47200>  C0235C6CH0 + NO3    = C0235C6CO3 + HNO3          : {%TrGTer} KNO3AL*5.5; {&2419}
<G47201>  C0235C6CH0 + OH     = C0235C6CO3                 : {%TrGTer} 6.70E-11; {&2419}
<G47202a> C0235C6CO3 + HO2    = C235C6CO3H                 : {%TrGTer} KAPH02*(rco3_ooh+rco3_o3); {&2419}
<G47202b> C0235C6CO3 + HO2    = C0235C6O2 + CO2 + OH       : {%TrGTer} KAPH02*rco3_oh; {&2419}
<G47203>  C0235C6CO3 + NO     = C0235C6O2 + CO2 + NO2      : {%TrGTer} KAPN0; {&2419}
<G47204>  C0235C6CO3 + NO2    = C7PAN3                     : {%TrGTer} k_CH3CO3_NO2; {&2419}
<G47205>  C0235C6CO3          = C0235C6O2 + CO2            : {%TrGTer} k1_R02RC03; {&2419}
<G47206>  C235C6CO3H + OH     = C0235C6CO3                 : {%TrGTer} 4.75E-12; {&2419}
<G47207>  C7PAN3 + OH         = C0235C5CH0 + CO + NO2      : {%TrGTer} 8.83E-13; {&2419}
<G47208>  C7PAN3              = C0235C6CO3 + NO2           : {%TrGTer} k_PAN_M; {&2419}
<G47209a> C7L602 + HO2        = C7L600H                    : {%TrGTer} KR02H02(7)*rcoch2o2_ooh; {&2419, 3031}
<G47209b> C7L602 + HO2        = C013C4CH0 + CH3CO + OH     : {%TrGTer} KR02H02(7)*rcoch2o2_oh; {&2419, 3031}
<G47210>  C7L602 + NO         = C013C4CH0 + CH3CO + NO2    : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G47211>  C7L602              = C013C4CH0 + CH3CO          : {%TrGTer} k1_R02s0R02; {&2419}
<G47212>  C7L600H + OH        = C0235C6CH0 + OH            : {%TrGTer} 1.20E-10; {&2419}
<G47213>  C72102 + HO2        = C72100H                    : {%TrGTer} KR02H02(7); {&2419}
<G47214>  C72102 + NO         = C72202 + NO2               : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G47215>  C72102              = C72202                     : {%TrGTer} k1_R02pR02; {&2419}
<G47216>  C72100H + OH        = C72102                     : {%TrGTer} 1.27E-11; {&2419}
<G47217>  C72202 + HO2        = C72200H                    : {%TrGTer} KR02H02(7); {&2419}
<G47218>  C72202 + NO         = CH3COCH3 + C4402 + NO2     : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G47219>  C72202              = CH3COCH3 + C4402           : {%TrGTer} k1_R02tR02; {&2419}
<G47220>  C72200H + OH        = C72202                     : {%TrGTer} 3.31E-11; {&2419}
<G47221>  R006R302            = R006R502                   : {%TrGTer} 5.60E10*EXP(-8745./TEMP); {&3019}
<G47222>  R006R302 + NO       = R006R30 + NO2              : {%TrGTer} KR02N0; {&3019} // \alkylnitrateneglected
<G47223>  R006R302 + HO2      = 7 LCARB0N                  : {%TrGTer} KR02H02(7); {&3019} // R006R300H produced but no sink for it.
<G47224>  R006R302            = R006R30                    : {%TrGTer} k1_R02sR02; {&3019}
<G47225>  R006R30             = 7 LCARB0N + HO2            : {%TrGTer} 5.7E10*EXP(-2949./TEMP); {&3019} // R006R4P produced but no sink for it.
<G47226>  R006R502            = 7 LCARB0N + OH             : {%TrGTer} 9.17E10*EXP(-8706./TEMP); {&3019} // R006R5P produced but no sink for it
<G47400>  TOLUENE    + OH     = .07 C6H5CH202 + .18 CRESOL + .18 HO2 + .65 TLBIPER02 + .10 TLEP0XMUC + .10 HO2 : {%TrGAro} 1.8E-12*EXP(340/TEMP); {&2419} // Merged.
<G47401>  C6H5CH202  + HO2    = C6H5CH200H                 : {%TrGAro} 1.5E-13*EXP(1310/TEMP); {&2419}
<G47402a> C6H5CH202  + NO     = C6H5CH2NO3                 : {%TrGAro} KR02N0*alpha_AN(7,1,0,0,0,temp,cair); {&2419} // KR0PRIM*02 fast reaction C6H5CH20 = BENZAL + HO2.
<G47402b> C6H5CH202  + NO     = BENZAL + HO2 + NO2         : {%TrGAro} KR02N0*(1.-alpha_AN(7,1,0,0,0,temp,cair)); {&2419} // KR0PRIM*02 fast reaction C6H5CH20 = BENZAL + HO2.
<G47403>  C6H5CH202  + NO3    = BENZAL + HO2 + NO2         : {%TrGAro} KR02NO3; {&2419} // KR0PRIM*02 fast reaction C6H5CH20 = BENZAL + HO2.
<G47404>  C6H5CH202           = BENZAL + HO2               : {%TrGAro} 2*(k_CH302*2.4E-14*EXP(1620./TEMP))**0.5*R02; {&2419} // KR0PRIM*02 fast reaction C6H5CH20 = BENZAL + HO2. C6H5CH20H replaced
with its oxidation product BENZAL.
<G47405>  CRESOL     + NO3    = .103 CRESO2 + .103 HNO3 + .506 NCRESO2 + .391 TOL10 + .391 HNO3 : {%TrGAro} 1.4E-11; {&2419} // Merged.
<G47406>  CRESOL     + OH     = .2 CRESO2 + .727 MCATECHOL + .727 HO2 + .073 TOL10              : {%TrGAro} 4.65E-11; {&2419} // Merged.
<G47407a> TLBIPER02  + HO2    = TLBIPER00H                                                                : {%TrGAro} KR02H02(7)*(1.-rbipero2_oh); {&2419}
<G47407b> TLBIPER02  + HO2    = OH + .6 GLYOX + .4 MGLYOX + HO2 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL : {%TrGAro} KR02H02(7)*rbipero2_oh; {&2419, 3188} // According to
\citet{3188}, the branching ratio rbipero2\_oh is set to 0.40 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.
<G47408a> TLBIPER02  + NO     = NO2 + .6 GLYOX + .4 MGLYOX + HO2 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL : {%TrGAro} KR02N0*(1.-alpha_AN(11,2,0,0,1,temp,cair)); {&2419} //
KDEC TLBIPER0 $\rightarrow$.6 GLYOX + .4 MGLYOX + HO2 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL
<G47408b> TLBIPER02  + NO     = TLBIPERN03                                    : {%TrGAro} KR02N0*alpha_AN(11,2,0,0,1,temp,cair); {&2419} // KDEC TLBIPER0 $\rightarrow$.6 GLYOX + .4 MGLYOX + HO2 + .2
ZC0DC23DB C0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL
<G47409>  TLBIPER02  + NO3    = NO2 + .6 GLYOX + .4 MGLYOX + HO2 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL : {%TrGAro} KR02NO3; {&2419} // KDEC TLBIPER0 $\rightarrow$.6 GLYOX +
.4 MGLYOX + HO2 + .2 ZC0DC23DB C0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL
<G47410>  TLBIPER02          = .6 GLYOX + .4 MGLYOX + HO2 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL       : {%TrGAro} k1_R02s0R02; {&2419} // Only major channel and KDEC
TLBIPER0 $\rightarrow$.6 GLYOX + .4 MGLYOX + HO2 + .2 ZC0DC23DB C0D + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL
<G47411>  TLEP0XMUC  + NO3    = TLEMUCC03 + HNO3           : {%TrGAro} KNO3AL*2.75; {&2419}
<G47412>  TLEP0XMUC  + O3     = EPXC4DIAL + .125 CH3CH0 + .695 CH3CO + .57 CO + .57 OH + .125 HO2 +.1125 CH3COCO2H + .0675 MGLYOX + .0675 H2O2  + .25 CO2 : {%TrGAro} 5.00E-18; {&2419} // KDEC MGL00B
$\rightarrow$ .125 CH3CH0 + .695 CH3CO + .57 CO + .57 OH + .125 HO2 + .18 MGL00 + .25 CO2
<G47413>  TLEP0XMUC  + OH     = .31 TLEMUCC03 + .69 TLEMUC02     : {%TrGAro} 7.99E-11; {&2419} // Merged.
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<G47414>  C6H5CH2OOH + OH     = BENZAL + OH                    : {%TrGAro} 2.05E-11; {&2419}
<G47415>  C6H5CH2NO3 + OH     = BENZAL + NO2                   : {%TrGAro} 6.03E-12; {&2419}
<G47416>  BENZAL     + NO3    = C6H5CO3 + HNO3                 : {%TrGAro} 2.40E-15; {&2419}
<G47417>  BENZAL     + OH     = C6H5CO3                        : {%TrGAro} 5.9E-12*EXP(225/TEMP); {&2419}
<G47418a> CRESO2     + HO2    = CRESOOH                        : {%TrGAro} KRO2HO2(7)*(1-rchohch2o2_oh); {&2419}
<G47418b> CRESO2     + HO2    = .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE + OH  : {%TrGAro} KRO2HO2(7)*rchohch2o2_oh; {&2419} // Reactions with KRO2HO2 and KDEC CRESO $\rightarrow$ .68 C5CO14OH + .68
GLYOX + HO2 + .32 PTLQ0NE.
<G47419>  CRESO2     + NO     = .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE + NO2 : {%TrGAro} KRO2NO; {&2419} // KDEC CRESO $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE
<G47420>  CRESO2     + NO3    = .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE + NO2 : {%TrGAro} KRO2NO3; {&2419} // KDEC CRESO $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE
<G47421>  CRESO2             = .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE       : {%TrGAro} kl_RO2IS0PD02; {&2419} // KDEC CRESO $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQ0NE and Only major
channel.
<G47422a> NCRESO2    + HO2    = NCRESOOH                       : {%TrGAro} KRO2HO2(7)*(1-rchohch2o2_oh); {&2419}
<G47422b> NCRESO2    + HO2    = C5CO14OH + GLYOX + NO2 + OH    : {%TrGAro} KRO2HO2(7)*rchohch2o2_oh; {&2419} // Reactions with KRO2HO2 and KDEC NCRESO $\rightarrow$ C5CO14OH + GLYOX + NO2
<G47423>  NCRESO2    + NO     = C5CO14OH + GLYOX + NO2 + NO2   : {%TrGAro} KRO2NO; {&2419} // KDEC NCRESO $\rightarrow$ C5CO14OH + GLYOX + NO2
<G47424>  NCRESO2    + NO3    = C5CO14OH + GLYOX + NO2 + NO2   : {%TrGAro} KRO2NO3; {&2419} // KDEC NCRESO $\rightarrow$ C5CO14OH + GLYOX + NO2
<G47425>  NCRESO2             = C5CO14OH + GLYOX + NO2         : {%TrGAro} kl_RO2IS0PD02; {&2419} // KDEC NCRESO $\rightarrow$ C5CO14OH + GLYOX + NO2 and Only major channel.
<G47426>  TOL10      + NO2    = TOL10HNO2                      : {%TrGAro} k_C6H50_NO2; {&2419, 3172} // {TOL10HNO2 is a nitro-phenol}
<G47427>  TOL10      + O3     = OXYL10Z                        : {%TrGAro} k_C6H50_O3; {&2419, 3171}
<G47428>  MCATECH0L  + NO3    = MCATEC10 + HNO3                : {%TrGAro} 1.7E-10*1.0; {&2419}
<G47429>  MCATECH0L  + O3     = MC30DBC02H + HCOC02H + HO2 + OH  : {%TrGAro} 2.8E-17; {&2419} // KDEC MCATEC00A $\rightarrow$ MC30DBC02H + HCOC02H + HO2 + OH
<G47430>  MCATECH0L  + OH     = MCATEC10                       : {%TrGAro} 2.0E-10*1.0; {&2419}
<G47431>  TLBIPER00H + OH     = TL0BIPER0H + OH                : {%TrGAro} 9.64E-11; {&2419}
<G47432>  TLBIPERN03 + OH     = TL0BIPER0H + NO2               : {%TrGAro} 7.16E-11; {&2419}
<G47433>  TL0BIPER0H + OH     = C5CO1402 + GLYOX               : {%TrGAro} 7.99E-11; {&2419}
<G47434a> TLEMUCC03  + HO2    = C615C0202 + CO2 + OH           : {%TrGAro} KAPH02*rco3_oh; {&2419}
<G47434b> TLEMUCC03  + HO2    = TLEMUCC02H + O3                : {%TrGAro} KAPH02*rco3_o3; {&2419}
<G47434c> TLEMUCC03  + HO2    = TLEMUCC03H                     : {%TrGAro} KAPH02*rco3_ooh; {&2419}
<G47435>  TLEMUCC03  + NO     = C615C0202  + CO2 + NO2         : {%TrGAro} KAPNO; {&2419}
<G47436>  TLEMUCC03  + NO2    = TLEMUCPAN                      : {%TrGAro} k_CH3C03_NO2; {&2419} // KFPAN $\rightarrow$k\_CH3C03\_NO2
<G47437>  TLEMUCC03  + NO3    = C615C0202  + CO2 + NO2         : {%TrGAro} KRO2NO3*1.74; {&2419}
<G47438>  TLEMUCC03           = C615C0202  + CO2               : {%TrGAro} kl_RO2RC03; {&2419} // Only major channel.
<G47439a> TLEMUC02   + HO2    = TLEMUC00H                      : {%TrGAro} KRO2HO2(7)*(1-rchohch2o2_oh-rcoch2o2_oh); {&2419}
<G47439b> TLEMUC02   + HO2    = .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02 + OH  : {%TrGAro} KRO2HO2(7)*(rchohch2o2_oh+rcoch2o2_oh); {&2419} // Reactions with KRO2HO2 and KDEC
TLEMUC0$\rightarrow$ .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02
<G47440a> TLEMUC02   + NO     = TLEMUCNO3                                                  : {%TrGAro} KRO2NO*alpha_AN(11,2,1,0,0,temp,cair); {&2419}
<G47440b> TLEMUC02   + NO     = .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02 + NO2 : {%TrGAro} KRO2NO*(1.-alpha_AN(11,2,1,0,0,temp,cair)); {&2419} // KDEC TLEMUC0$\rightarrow$ .5 C3DIAL02 +
.5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02
<G47441>  TLEMUC02   + NO3    = .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02 + NO2 : {%TrGAro} KRO2NO3; {&2419} // KDEC TLEMUC0$\rightarrow$ .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5
MGLY0X + .5 H02
<G47442>  TLEMUC02            = .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02       : {%TrGAro} kl_RO2s0RO2; {&2419} // KDEC TLEMUC0$\rightarrow$ .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL +
.5 MGLY0X + .5 H02 and Only major channel.
<G47443a> C6H5CO3    + HO2    = C6H5CO3H                       : {%TrGAro} 1.1E-11*EXP(364./temp)*0.65 ; {&3201}
<G47443b> C6H5CO3    + HO2    = C6H5O2 + CO2 + OH              : {%TrGAro} 1.1E-11*EXP(364./temp)*0.20 ; {&3201}
<G47443c> C6H5CO3    + HO2    = PHCOOH + O3                    : {%TrGAro} 1.1E-11*EXP(364./temp)*0.15 ; {&3201}
<G47444>  C6H5CO3    + NO     = C6H5O2 + CO2 + NO2             : {%TrGAro} KAPNO; {&2419}
<G47445>  C6H5CO3    + NO2    = PBZN                           : {%TrGAro} k_CH3C03_NO2; {&2419} // KFPAN $\rightarrow$k\_CH3C03\_NO2
<G47446>  C6H5CO3    + NO3    = C6H5O2 + CO2 + NO2             : {%TrGAro} KRO2NO3*1.74; {&2419}
<G47447>  C6H5CO3             = C6H5O2 + CO2                   : {%TrGAro} kl_RO2RC03; {&2419} // Only major channel.
<G47448>  CRESOOH    + OH     = CRESO2                         : {%TrGAro} 1.15E-10; {&2419}
<G47449>  NCRESOOH   + OH     = NCRESO2                        : {%TrGAro} 1.07E-10; {&2419}
<G47450>  TOL10HNO2  + NO3    = NCRES10 + HNO3                 : {%TrGAro} 3.13E-13*1.0; {&2419}
<G47451>  TOL10HNO2  + OH     = NCRES10                        : {%TrGAro} 2.8E-12; {&2419}
<G47452>  OXYL10Z    + HO2    = OXYL10OH                       : {%TrGAro} KRO2HO2(7); {&2419}
<G47453>  OXYL10Z    + NO     = TOL10 + NO2                    : {%TrGAro} KRO2NO; {&2419}
<G47454>  OXYL10Z    + NO2    = TOL10 + NO3                    : {%TrGAro} K_C6H5O2_NO2; {&3167} // New channel.
<G47455>  OXYL10Z    + NO3    = TOL10 + NO2                    : {%TrGAro} KRO2NO3; {&2419}
<G47456>  OXYL10Z             = TOL10                          : {%TrGAro} kl_RO2sRO2; {&2419}
<G47457>  MCATEC10   + NO2    = MNCATECH                       : {%TrGAro} k_C6H50_NO2; {&2419, 3172}
<G47458>  MCATEC10   + O3     = MCATEC102                      : {%TrGAro} k_C6H50_O3; {&2419, 3171}
<G47459>  TLEMUCC02H + OH     = C615C0202 + CO2                : {%TrGAro} 5.98E-11; {&2419}
<G47460>  TLEMUCC03H + OH     = TLEMUCC03                      : {%TrGAro} 6.29E-11; {&2419}
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<G47461>  TLEMUCPAN  + OH     = C5DICARB + CO + CO2 + NO2        : {%TrGAro} 5.96E-11; {&2419}
<G47462>  TLEMUCPAN           = TLEMUCO3 + NO2                   : {%TrGAro} k_PAN_M; {&2419}
<G47463>  TLEMUCOOH  + OH     = TLEMUCCO + OH                    : {%TrGAro} 7.04E-11; {&2419}
<G47464>  TLEMUCNO3  + OH     = TLEMUCCO + NO2                   : {%TrGAro} 3.06E-11; {&2419}
<G47465>  TLEMUCCO   + OH     = CH3CO + EPXC4DIAL + CO           : {%TrGAro} 4.06E-11; {&2419}
<G47466>  C6H5CO3H   + OH     = C6H5CO3                          : {%TrGAro} 4.66E-12; {&2419}
<G47467>  PHCOOH     + OH     = C6H5O2 + CO2                     : {%TrGAro} 1.10E-12; {&2419}
<G47468>  PBZN       + OH     = C6H5OOH + CO + NO2               : {%TrGAro} 1.06E-12; {&2419}
<G47469>  PBZN                = C6H5CO3 + NO2                    : {%TrGAro} k_PAN_M*0.67; {&2419}
<G47470>  PTLQONE    + NO3    = NPTLQO2                          : {%TrGAro} 1.00E-12; {&2419}
<G47471>  PTLQONE    + OH     = PTLQO2                           : {%TrGAro} 2.3E-11; {&2419}
<G47472>  NCRES10    + NO2    = DNCRES                           : {%TrGAro} k_C6H5O_NO2; {&2419, 3172}
<G47473>  NCRES10    + O3     = NCRES10O2                        : {%TrGAro} k_C6H5O_O3; {&2419, 3171}
<G47474>  OXYL1OOH   + OH     = OXYL1O2                          : {%TrGAro} 4.65E-11; {&2419}
<G47475>  MNCATECH   + NO3    = MNNCATECO2                       : {%TrGAro} 5.03E-12; {&2419}
<G47476>  MNCATECH   + OH     = MNCATECO2                        : {%TrGAro} 6.83E-12; {&2419}
<G47477>  MCATEC1O2  + HO2    = MCATEC1OOH                       : {%TrGAro} KR02H02(7); {&2419}
<G47478>  MCATEC1O2  + NO     = MCATEC1O + NO2                   : {%TrGAro} KR02NO; {&2419}
<G47479>  MCATEC1O2  + NO2    = MCATEC1O + NO3                   : {%TrGAro} K_C6H5O2_NO2; {&3167} // New channel.
<G47480>  MCATEC1O2  + NO3    = MCATEC1O + NO2                   : {%TrGAro} KR02NO3; {&2419}
<G47481>  MCATEC1O2           = MCATEC1O                         : {%TrGAro} k1_R02s0R02; {&2419}
<G47482a> NPTLQO2    + HO2    = NPTLQOOH                         : {%TrGAro} KR02H02(7)*(1-rcoch2o2_oh); {&2419}
<G47482b> NPTLQO2    + HO2    = C7C04DB + NO2 + OH               : {%TrGAro} KR02H02(7)*rcoch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC NPTLQ0 $\rightarrow$ C7C04DB + NO2
<G47483>  NPTLQO2    + NO     = C7C04DB + NO2 + NO2              : {%TrGAro} KR02NO; {&2419} // KDEC NPTLQ0 $\rightarrow$ C7C04DB + NO2
<G47484>  NPTLQO2    + NO3    = C7C04DB + NO2 + NO2              : {%TrGAro} KR02NO3; {&2419} // KDEC NPTLQ0 $\rightarrow$ C7C04DB + NO2
<G47485>  NPTLQO2             = C7C04DB + NO2                    : {%TrGAro} k1_R02s0R02; {&2419} // KDEC NPTLQ0 $\rightarrow$ C7C04DB + NO2
<G47486a> PTLQO2     + HO2    = PTLQOOH                          : {%TrGAro} KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh); {&2419}
<G47486b> PTLQO2     + HO2    = C6C020HC03 + OH                  : {%TrGAro} KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh); {&2419} // Reactions with KR02H02 and KDEC PTLQ0 $\rightarrow$ C6C020HC03
<G47487>  PTLQO2     + NO     = C6C020HC03 + NO2                 : {%TrGAro} KR02NO; {&2419} // KDEC PTLQ0 $\rightarrow$ C6C020HC03
<G47488>  PTLQO2     + NO3    = C6C020HC03 + NO2                 : {%TrGAro} KR02NO3; {&2419} // KDEC PTLQ0 $\rightarrow$ C6C020HC03
<G47489>  PTLQO2              = C6C020HC03                       : {%TrGAro} k1_R02s0R02; {&2419} // Only major channel. KDEC PTLQ0 $\rightarrow$ C6C020HC03.
<G47490>  DNCRES     + NO3    = NDNCRES02                        : {%TrGAro} 7.83E-15; {&2419}
<G47491>  DNCRES     + OH     = DNCRES02                         : {%TrGAro} 5.10E-14; {&2419}
<G47492>  NCRES1O2   + HO2    = NCRES1OOH                        : {%TrGAro} KR02H02(7); {&2419}
<G47493>  NCRES1O2   + NO     = NCRES1O + NO2                    : {%TrGAro} KR02NO; {&2419}
<G47494>  NCRES1O2   + NO2    = NCRES1O + NO3                    : {%TrGAro} K_C6H5O2_NO2; {&3167} // New channel.
<G47495>  NCRES1O2   + NO3    = NCRES1O + NO2                    : {%TrGAro} KR02NO3; {&2419}
<G47496>  NCRES1O2            = NCRES1O                          : {%TrGAro} k1_R02sR02; {&2419}
<G47497a> MNNCATECO2 + HO2    = MNNCATCOOH                       : {%TrGAro} KR02H02(7)*(1-rchohch2o2_oh); {&2419}
<G47497b> MNNCATECO2 + HO2    = NC4MDCO2H + HCOCO2H + NO2 + OH   : {%TrGAro} KR02H02(7)*rchohch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC MNNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
<G47498>  MNNCATECO2 + NO     = NC4MDCO2H + HCOCO2H + NO2 + NO2  : {%TrGAro} KR02NO; {&2419} // KDEC MNNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
<G47499>  MNNCATECO2 + NO3    = NC4MDCO2H + HCOCO2H + NO2 + NO2  : {%TrGAro} KR02NO3; {&2419} // KDEC MNNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
<G47500>  MNNCATECO2          = NC4MDCO2H + HCOCO2H + NO2        : {%TrGAro} k1_R02IS0PD02; {&2419}
<G47501a> MNCATECO2  + HO2    = MNCATECOOH                       : {%TrGAro} KR02H02(7)*(1-rchohch2o2_oh); {&2419}
<G47501b> MNCATECO2  + HO2    = NC4MDCO2H + HCOCO2H + HO2 + OH   : {%TrGAro} KR02H02(7)*rchohch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC MNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + HO2
<G47502>  MNCATECO2  + NO     = NC4MDCO2H + HCOCO2H + HO2 + NO2  : {%TrGAro} KR02NO; {&2419} // KDEC MNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + HO2
<G47503>  MNCATECO2  + NO3    = NC4MDCO2H + HCOCO2H + HO2 + NO2  : {%TrGAro} KR02NO3; {&2419} // KDEC MNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + HO2
<G47504>  MNCATECO2           = NC4MDCO2H + HCOCO2H + HO2        : {%TrGAro} k1_R02IS0PD02; {&2419} // KDEC MNCATEC0 $\rightarrow$ NC4MDCO2H + HCOCO2H + HO2
<G47505>  MCATEC1OOH + OH     = MCATEC1O2                        : {%TrGAro} 2.05E-10; {&2419}
<G47506>  NPTLQOOH   + OH     = NPTLQO2                          : {%TrGAro} 8.56E-11; {&2419}
<G47507>  PTLQOOH    + OH     = PTLQCO + OH                      : {%TrGAro} 1.42E-10; {&2419}
<G47508>  PTLQCO     + OH     = C6C020HC03                       : {%TrGAro} 7.95E-11; {&2419}
<G47509a> NDNCRES02  + HO2    = NDNCRES00H                       : {%TrGAro} KR02H02(7)*(1-rchohch2o2_oh); {&2419}
<G47509b> NDNCRES02  + HO2    = NC4MDCO2H + HNO3 + 2 CO + NO2 + OH  : {%TrGAro} KR02H02(7)*rchohch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC NDNCRES0 $\rightarrow$ NC4MDCO2H + HNO3 + CO + CO + NO2
<G47510>  NDNCRES02  + NO     = NC4MDCO2H + HNO3 + 2 CO + NO2 + NO2 : {%TrGAro} KR02NO; {&2419} // KDEC NDNCRES0 $\rightarrow$ NC4MDCO2H + HNO3 + CO + CO + NO2
<G47511>  NDNCRES02  + NO3    = NC4MDCO2H + HNO3 + 2 CO + NO2 + NO2 : {%TrGAro} KR02NO3; {&2419} // KDEC NDNCRES0 $\rightarrow$ NC4MDCO2H + HNO3 + CO + CO + NO2
<G47512>  NDNCRES02           = NC4MDCO2H + HNO3 + 2 CO + NO2    : {%TrGAro} k1_R02IS0PD02; {&2419} // KDEC NDNCRES0 $\rightarrow$ NC4MDCO2H + HNO3 + CO + CO + NO2
<G47513a> DNCRES02   + HO2    = DNCRES00H                        : {%TrGAro} KR02H02(7)*(1-rchohch2o2_oh); {&2419}
<G47513b> DNCRES02   + HO2    = NC4MDCO2H + HCOCO2H + NO2 + OH   : {%TrGAro} KR02H02(7)*rchohch2o2_oh; {&2419} // Reactions with KR02H02 and KDEC DNCRES0 $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
<G47514>  DNCRES02   + NO     = NC4MDCO2H + HCOCO2H + NO2 + NO2  : {%TrGAro} KR02NO; {&2419} // KDEC DNCRES0 $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
<G47515>  DNCRES02   + NO3    = NC4MDCO2H + HCOCO2H + NO2 + NO2  : {%TrGAro} KR02NO3; {&2419} // KDEC DNCRES0 $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
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<G47516>  DNCRES02           = NC4MDC02H + HC0C02H + N02        : {%TrGAro} k1_R02IS0PD02; {&2419} // KDEC DNCRES0 $\rightarrow$ NC4MDC02H + HC0C02H + N02
<G47517>  NCRES100H  + 0H    = NCRES102                         : {%TrGAro} 1.53E-12; {&2419}
<G47518>  MNNCATC00H + 0H    = MNNCATEC02                       : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G47519>  MNCATEC00H + 0H    = MNCATEC02                        : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G47520>  C7C04DB    + 0H    = C0 + C0 + CH3C0 + C33C0          : {%TrGAro} 9.58E-11; {&2419}
<G47521a> C6C020HC03 + H02   = C5134C020H + H02 + C0 + C02 + 0H : {%TrGAro} KAPH02*rco3_oh; {&2419}
<G47521b> C6C020HC03 + H02   = C6C00HC03H                       : {%TrGAro} KAPH02*(rco3_ooh+rco3_o3); {&2419}
<G47522>  C6C020HC03 + N0    = C5134C020H + H02 + C0 + C02 + N02 : {%TrGAro} KAPN0; {&2419}
<G47523>  C6C020HC03 + N02   = C6C020HPAN                       : {%TrGAro} k_CH3C03_N02; {&2419}
<G47524>  C6C020HC03 + N03   = C5134C020H + H02 + C0 + C02 + N02 : {%TrGAro} KR02N03*1.74; {&2419}
<G47525>  C6C020HC03         = C5134C020H + H02 + C0 + C02      : {%TrGAro} k1_R02RC03; {&2419}
<G47526>  NDNCRES00H + 0H    = NDNCRES02                        : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G47527>  DNCRES00H  + 0H    = DNCRES02                         : {%TrGAro} 0.6*k_CH300H_0H; {&2419}
<G47528>  C6C00HC03H + 0H    = C6C020HC03                       : {%TrGAro} 9.29E-11; {&2419}
<G47529>  C6C020HPAN + 0H    = C5134C020H + C0 + C0 + N02       : {%TrGAro} 8.96E-11; {&2419}
<G47530>  C6C020HPAN         = C6C020HC03 + N02                 : {%TrGAro} k_PAN_M; {&2419}
<G48200>  C8502              = C8602                            : {%TrGTer} k1_R02tR02; {&2419}
<G48201>  C8502 + H02        = C8500H                           : {%TrGTer} KR02H02(8); {&2419}
<G48202>  C8502 + N0         = C8602 + N02                      : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G48203>  C8500H + 0H        = C8502                            : {%TrGTer} 1.29E-11; {&2419}
<G48204>  C8602              = C5102 + CH3C0CH3                 : {%TrGTer} k1_R02tR02; {&2419}
<G48205>  C8602 + N0         = C5102 + CH3C0CH3 + N02           : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G48206>  C8602 + H02        = C8600H                           : {%TrGTer} KR02H02(8); {&2419}
<G48207>  C8600H + 0H        = C8602                            : {%TrGTer} 3.45E-11; {&2419}
<G48208>  C81102             = C81202                           : {%TrGTer} k1_R02pR02; {&2419}
<G48209>  C81102 + H02       = 8 LCARB0N                        : {%TrGTer} KR02H02(8); {&2419}
<G48210>  C81102 + N0        = C81202      + N02                : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G48211>  C81202             = C81302                           : {%TrGTer} k1_R02t0R02; {&2419}
<G48212>  C81202 + N0        = C81302 + N02                     : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G48213>  C81202 + H02       = C81200H                          : {%TrGTer} KR02H02(8); {&2419}
<G48214>  C81200H + 0H       = C81202                           : {%TrGTer} 1.09E-11; {&2419}
<G48215>  C81302             = CH3C0CH3 + C51202                : {%TrGTer} k1_R02tR02; {&2419}
<G48216>  C81302 + N0        = CH3C0CH3 + C51202 + N02          : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G48217>  C81302 + H02       = C81300H                          : {%TrGTer} KR02H02(8); {&2419}
<G48218>  C81300H + 0H       = C81302                           : {%TrGTer} 1.86E-11; {&2419}
<G48219>  C721CH0 + N03      = C721C03 + HN03                   : {%TrGTer} KN03AL*8.5; {&2419}
<G48220>  C721CH0 + 0H       = C721C03                          : {%TrGTer} 2.63E-11; {&2419}
<G48221a> C721C03 + H02      = C721C03H                         : {%TrGTer} KAPH02*rco3_ooh; {&2419}
<G48221b> C721C03 + H02      = C72102 + C02 + 0H                : {%TrGTer} KAPH02*rco3_oh; {&2419}
<G48221c> C721C03 + H02      = N0RPINIC + 03                    : {%TrGTer} KAPH02*rco3_o3; {&2419}
<G48222>  C721C03 + N0       = C72102 + C02 + N02               : {%TrGTer} KAPN0; {&2419} // \alkylnitrateneglected
<G48223>  C721C03 + N02      = C721PAN                          : {%TrGTer} k_CH3C03_N02; {&2419}
<G48224>  C721C03 + N03      = C72102 + C02 + N02               : {%TrGTer} KR02N03*1.74; {&2419}
<G48225>  C721C03            = C72102 + C02                     : {%TrGTer} k1_R02RC03*0.9; {&3031}
<G48226>  C721C03            = N0RPINIC                         : {%TrGTer} k1_R02RC03*0.1; {&3031}
<G48227>  C721C03H + 0H      = C721C03                          : {%TrGTer} 9.65E-12; {&2419}
<G48228>  N0RPINIC + 0H      = C72102 + C02                     : {%TrGTer} 6.57E-12; {&2419}
<G48229>  C721PAN + 0H       = C72100H + C0 + N02               : {%TrGTer} 2.96E-12; {&2419}
<G48230>  C721PAN            = C721C03 + N02                    : {%TrGTer} k_PAN_M; {&2419}
<G48231>  C8BC + 0H          = C8BC02                           : {%TrGTer} 3.04E-12; {&2419}
<G48232>  C8BC02 + H02       = C8BC00H                          : {%TrGTer} KR02H02(8); {&2419}
<G48233a> C8BC02 + N0        = C8902 + N02                      : {%TrGTer} KR02N0*(1.-alpha_AN(8,2,0,0,0,temp,cair)); {&2419}
<G48233b> C8BC02 + N0        = C8BCN03                          : {%TrGTer} KR02N0*alpha_AN(8,2,0,0,0,temp,cair); {&2419}
<G48234>  C8BC02             = C8902                            : {%TrGTer} k1_R02sR02; {&2419}
<G48235>  C8BC00H + 0H       = C8BCC0 + 0H                      : {%TrGTer} 1.62E-11; {&2419}
<G48236>  C8BCN03 + 0H       = C8BCC0 + N02                     : {%TrGTer} 1.84E-12; {&2419}
<G48237>  C8BCC0 + 0H        = C8902                            : {%TrGTer} 3.94E-12; {&2419}
<G48238>  C8902 + H02        = C8900H                           : {%TrGTer} KR02H02(8); {&2419}
<G48239a> C8902 + N0         = C81002 + N02                     : {%TrGTer} KR02N0*(1.-alpha_AN(7,2,0,0,0,temp,cair)); {&2419}
<G48239b> C8902 + N0         = C89N03                           : {%TrGTer} KR02N0*alpha_AN(7,2,0,0,0,temp,cair); {&2419}
<G48240>  C8902 + N03        = C81002 + N02                     : {%TrGTer} KR02N03; {&2419}
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<G48241>  C8H02              = C81OO2                          : {%TrGTer} k1_RO2tRO2; {&2419}
<G48242>  C8H00H + OH        = C8H02                           : {%TrGTer} 3.61E-11; {&2419}
<G48243>  C8HNO3 + OH        = CH3COCH3 + CO13C4CHO + NO2      : {%TrGTer} 2.56E-11; {&2419}
<G48244>  C81OO2 + HO2       = C81OOOH                         : {%TrGTer} KRO2HO2(8); {&2419}
<G48245a> C81OO2 + NO        = CH3COCH3 + C51402 + NO2         : {%TrGTer} KRO2NO*(1.-alpha_AN(10,3,0,0,0,temp,cair)); {&2419}
<G48245b> C81OO2 + NO        = C81ONO3                         : {%TrGTer} KRO2NO*alpha_AN(10,3,0,0,0,temp,cair); {&2419}
<G48246>  C81OO2 + NO3       = CH3COCH3 + C51402 + NO2         : {%TrGTer} KRO2NO3; {&2419}
<G48247>  C81OO2             = CH3COCH3 + C51402               : {%TrGTer} k1_RO2tRO2; {&2419}
<G48248>  C81OOOH + OH       = C81OO2                          : {%TrGTer} 8.35E-11; {&2419}
<G48249>  C81ONO3 + OH       = CH3COCH3 + CO13C4CHO + NO2      : {%TrGTer} 4.96E-11; {&2419}
<G48400a> LXYL       + OH    = TLEPOXMUC + HO2  + LCARBON      : {%TrGAro} O.401E-11; {&2419} // Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (1.36E-11*0.24 + 2.31E-11*0.29 + 1.43E-11*0.155)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.
<G48400b> LXYL       + OH    = CLH5CH202       + LCARBON       : {%TrGAro} O.101E-11; {&2419} // Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (1.36E-11*0.05 + 2.31E-11*0.04 + 1.43E-11*0.10)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.
<G48400c> LXYL       + OH    = CRESOL          + LCARBON       : {%TrGAro} O.261E-11; {&2419} // Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (1.36E-11*0.16 + 2.31E-11*0.17 + 1.43E-11*0.12)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.
<G48400d> LXYL       + OH    = TLBIPER02 +  HO2 + LCARBON      : {%TrGAro} O.932E-11; {&2419} // Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (1.36E-11*0.55 + 2.31E-11*0.50 + 1.43E-11*0.625)/3, where k and coefficients are for the single isomers ortho, meta and para from MCM.
<G48401>  LXYL       + NO3   = CLH5CH202 + HNO3 + LCARBON      : {%TrGAro} 3.9E-16; {&2419} // Same products as for toluene. The rate constant is the average of m, p, o k=(4.10E-16+2.60E-16+5.00E-16)/3 =
3.9E-16.
<G48402>  EBENZ      + OH    = .10 TLEPOXMUC + .07 CLH5CH202 + .18 CRESOL + .65 TLBIPER02 + .28 HO2 + LCARBON : {%TrGAro} 7.00E-12; {&2419} // merged under same rate constant
<G48403>  EBENZ      + NO3   = CLH5CH202 + HNO3 + LCARBON      : {%TrGAro} 1.20E-16; {&2419} // Same products as for toluene
<G48404>  STYRENE    + NO3   = NSTYREN02                       : {%TrGAro} 1.50E-12; {&2419}
<G48405>  STYRENE    + O3    = .545 HCHO + .1 BENZENE + .28 CLH502 + .56 CO + .36 OH + .28 HO2 + .075 PHCOOH + .545 BENZAL +  .09 H202 + .075 HCOOH + .2 CO2 : {%TrGAro} 1.70E-17; {&2419} // KDEC CH200B
$\rightarrow$ .24 CH200 + .40 CO + .36 HO2 + .36 CO + .36 OH and  H20subs PHCHOO $\rightarrow$ .625 PHCOOH + .375 BENZAL + .375 H202 + .2 CO2
<G48406>  STYRENE    + OH    = STYREN02                        : {%TrGAro} 5.80E-11; {&2419}
<G48407>  NSTYREN02  + HO2   = NSTYREN00H                      : {%TrGAro} KRO2HO2(8); {&2419}
<G48408>  NSTYREN02  + NO    = NO2 + NO2 + HCHO + BENZAL       : {%TrGAro} KRO2NO; {&2419} // KDEC NSTYRENE0 $\rightarrow$ NO2 + HCHO + BENZAL
<G48409>  NSTYREN02  + NO3   = NO2 + NO2 + HCHO + BENZAL       : {%TrGAro} KRO2NO3; {&2419} // KDEC NSTYRENE0 $\rightarrow$ NO2 + HCHO + BENZAL
<G48410>  NSTYREN02          = NO2 + HCHO + BENZAL             : {%TrGAro} k1_RO2sRO2; {&2419} // KDEC NSTYRENE0 $\rightarrow$ NO2 + HCHO + BENZAL
<G48411>  NSTYREN00H + OH    = NSTYREN02                       : {%TrGAro} 6.16E-11; {&2419}
<G48412a> STYREN02   + HO2   = STYREN00H                       : {%TrGAro} KRO2HO2(8)*(1-rchohch2o2_oh); {&2419}
<G48412b> STYREN02   + HO2   = HO2 + OH + HCHO + BENZAL        : {%TrGAro} KRO2HO2(8)*rchohch2o2_oh; {&2419} // KDEC STYREN0 $\rightarrow$ HO2 + HCHO + BENZAL and reactions with KRO2HO2.
<G48413>  STYREN02   + NO    = NO2 + HO2 + HCHO + BENZAL       : {%TrGAro} KRO2NO; {&2419} // KDEC STYREN0 $\rightarrow$ HO2 + HCHO + BENZAL
<G48414>  STYREN02   + NO3   = NO2 + HO2 + HCHO + BENZAL       : {%TrGAro} KRO2NO3; {&2419} // KDEC STYREN0 $\rightarrow$ HO2 + HCHO + BENZAL
<G48415>  STYREN02           = HO2 + HCHO + BENZAL             : {%TrGAro} k1_RO2sRO2; {&2419} // KDEC STYREN0 $\rightarrow$ HO2 + HCHO + BENZAL
<G48416>  STYREN00H  + OH    = STYREN02                        : {%TrGAro} 6.16E-11; {&2419}
<G49200>  C96O2              = C97O2                           : {%TrGTer} k1_RO2pRO2; {&2419}
<G49201>  C96O2 + HO2        = C96OOH                          : {%TrGTer} KRO2HO2(9); {&2419}
<G49202a> C96O2 + NO         = C97O2 + NO2                     : {%TrGTer} KRO2NO*(1.-alpha_AN(10,1,0,0,0,temp,cair)); {&2419}
<G49202b> C96O2 + NO         = C96NO3                          : {%TrGTer} KRO2NO*alpha_AN(10,1,0,0,0,temp,cair); {&2419}
<G49203>  C96NO3 + OH        = NORPINAL + NO2                  : {%TrGTer} 2.88E-12; {&2419}
<G49204a> C96OOH + OH        = C96O2                           : {%TrGTer} O.6*k_CH3OOH_OH; {&2419}
<G49205b> C96OOH + OH        = NORPINAL + OH                   : {%TrGTer} 1.30E-11; {&2419}
<G49206>  C97O2              = C98O2                           : {%TrGTer} k1_RO2tRO2; {&2419}
<G49207>  C97O2 + NO         = C98O2 + NO2                     : {%TrGTer} KRO2NO; {&2419} // \alkylnitrateneglected
<G49208a> C97O2 + HO2        = C97OOH                          : {%TrGTer} KRO2HO2(9)*rcoch2o2_ooh; {&2419, 3031}
<G49208b> C97O2 + HO2        = C98O2 + OH                      : {%TrGTer} KRO2HO2(9)*rcoch2o2_oh; {&2419, 3031}
<G49209>  C97OOH + OH        = C97O2                           : {%TrGTer} 1.05E-11; {&2419}
<G49210>  C98O2              = CL1402 + CH3COCH3               : {%TrGTer} k1_RO2tRO2; {&2419}
<G49211a> C98O2 + NO         = CL1402 + CH3COCH3 + NO2         : {%TrGTer} KRO2NO*(1.-alpha_AN(12,3,0,0,0,temp,cair)); {&2419}
<G49211b> C98O2 + NO         = 9 LCARBON + LNITROGEN           : {%TrGTer} KRO2NO*alpha_AN(12,3,0,0,0,temp,cair); {&2419}
<G49212>  C98O2 + HO2        = C98OOH                          : {%TrGTer} KRO2HO2(9); {&2419}
<G49213>  C98OOH + OH        = C98O2                           : {%TrGTer} 2.05E-11; {&2419}
<G49214>  NORPINAL + OH      = C85CO3                          : {%TrGTer} 2.64E-11; {&2419}
<G49215>  NORPINAL + NO3     = C85CO3 + HNO3                   : {%TrGTer} KNO3AL*8.5; {&2419}
<G49216>  C85CO3             = C8502 + CO2                     : {%TrGTer} k1_RO2RCO3; {&2419}
<G49217>  C85CO3 + NO        = C8502 + CO2 + NO2               : {%TrGTer} KAPNO; {&2419}
<G49218>  C85CO3 + NO2       = C9PAN2                          : {%TrGTer} k_CH3CO3_NO2; {&2419}
<G49219a> C85CO3 + HO2       = C85CO3H                         : {%TrGTer} KAPHO2*(rco3_ooh+rco3_o3); {&2419}
<G49219b> C85CO3 + HO2       = C8502 + CO2 + OH                : {%TrGTer} KAPHO2*rco3_oh; {&2419}
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<G49220>  C9PAN2              = C85C03 + N02                    : {%TrGTer} k_PAN_M; {&2419}
<G49221>  C9PAN2 + OH         = C8500H + C0 + N02               : {%TrGTer} 6.60E-12; {&2419}
<G49222>  C85C03H + OH        = C85C03                          : {%TrGTer} 1.02E-11; {&2419}
<G49223a> C89C03              = .8 C811C03 + .2 C8902 + .2 C02  : {%TrGTer} k1_R02RC03*0.9; {&3031}
<G49223b> C89C03              = C89C02H                         : {%TrGTer} k1_R02RC03*0.1; {&3031}
<G49224a> C89C03 + H02        = C89C03H                         : {%TrGTer} KAPH02*rco3_ooh; {&2419}
<G49224b> C89C03 + H02        = C89C02H + 03                    : {%TrGTer} KAPH02*rco3_o3; {&2419}
<G49224c> C89C03 + H02        = .80 C811C03 + .20 C8902 + .2 C02 + 0H : {%TrGTer} KAPH02*rco3_oh; {&2419}
<G49225>  C89C03 + N02        = C89PAN                          : {%TrGTer} k_CH3C03_N02; {&2419}
<G49226>  C89C03 + N0         = .8 C811C03 + .2 C8902 + .2 C02 + N02 : {%TrGTer} KAPN0; {&2419}
<G49227>  C89C02H + 0H        = .8 C811C03 + .2 C8902 + .2 C02  : {%TrGTer} 2.69E-11; {&2419}
<G49228>  C89C03H + 0H        = C89C03                          : {%TrGTer} 3.00E-11; {&2419}
<G49229>  C89PAN              = C89C03 + N02                    : {%TrGTer} k_PAN_M; {&2419}
<G49230>  C89PAN + 0H         = CH3C0CH3 + C013C4CH0 + C0 + N02 : {%TrGTer} 2.52E-11; {&2419}
<G49231a> C811C03             = C8110Z + C02                    : {%TrGTer} k1_R02RC03*0.9; {&3031}
<G49231b> C811C03             = PINIC                           : {%TrGTer} k1_R02RC03*0.1; {&3031}
<G49232a> C811C03 + H02       = C811C03H                        : {%TrGTer} KAPH02*rco3_ooh; {&2419}
<G49232b> C811C03 + H02       = PINIC + 03                      : {%TrGTer} KAPH02*rco3_o3; {&2419}
<G49232c> C811C03 + H02       = C8110Z + C02 + 0H               : {%TrGTer} KAPH02*rco3_oh; {&2419}
<G49233>  C811C03 + N0        = C8110Z + C02 + N02              : {%TrGTer} KAPN0; {&2419}
<G49234>  C811C03 + N02       = C811PAN                         : {%TrGTer} k_CH3C03_N02; {&2419}
<G49235>  PINIC + 0H          = C8110Z + C02                    : {%TrGTer} 7.29E-12; {&2419}
<G49236>  N0PIN0NE + 0H       = N0PIND02                        : {%TrGTer} 1.55E-11; {&3028, 2419}
<G49237a> N0PIND02 + H02      = N0PIND00H                       : {%TrGTer} KR02H02(9)*rcoch2o2_ooh; {&2419, 3031}
<G49237b> N0PIND02 + H02      = C89C03 + 0H                     : {%TrGTer} KR02H02(9)*rcoch2o2_oh; {&2419, 3031}
<G49238>  N0PIND02 + N0       = C89C03 + N02                    : {%TrGTer} KR02N0; {&2419} // \alkylnitrateneglected
<G49239>  N0PIND02            = C89C03                          : {%TrGTer} k1_R02p0R02; {&2419}
<G49240>  N0PIND00H {+ 0H}    = N0PINDC0 {+ 0H}                 : {%TrGTer} 2.63E-11; {&2419}
<G49241>  N0PINDC0 + 0H       = C89C03                          : {%TrGTer} 3.07E-12; {&2419}
<G49242>  N0PIN00             = N0PIN0NE + H202                 : {%TrGTer} 6.00E-18*c(ind_H20); {&2419}
<G49243>  N0PIN00 + C0        = N0PIN0NE + C02                  : {%TrGTer} 1.2E-15; {&2419}
<G49244>  N0PIN00 + N0        = N0PIN0NE + N02                  : {%TrGTer} 1.E-14; {&2419}
<G49245>  N0PIN00 + N02       = N0PIN0NE + N03                  : {%TrGTer} 1.E-15; {&2419}
<G49246>  N0RPINEN0L + 0H     = HC00H + 0H + C8602              : {%TrGTer} k_CH2CH0H_0H_HC00H; {&3031, 3179} // \onlythischannel Instead of the (lacking) carbonyl a product of further degradation is
assumed.
<G49247>  N0RPINEN0L + HC00H  = N0RPINAL + HC00H                : {%TrGTer} k_CH2CH0H_HC00H; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G49248>  N0RPINAL  + HC00H   = N0RPINEN0L + HC00H              : {%TrGTer} k_ALD_HC00H; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G49249>  C811C03H + 0H       = C811C03                         : {%TrGTer} 1.04E-11; {&2419}
<G49250>  C811PAN             = C811C03 + N02                   : {%TrGTer} k_PAN_M; {&2419}
<G49251>  C811PAN + 0H        = C721CH0 + C0 + N02              : {%TrGTer} 6.77E-12; {&2419}
<G49400a> LTMB       + 0H     = TLEP0XMUC + H02  + 2 LCARB0N    : {%TrGAro} 0.827E-11; {&2419} // Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (3.27E-11*0.21 + 3.25E-11*0.30 + 5.67E-11*0.14)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.
<G49400b> LTMB       + 0H     = C6H5CH202        + 2 LCARB0N    : {%TrGAro} 0.189E-11; {&2419} // Same products as for toluene . Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (3.27E-11*0.06 + 3.25E-11*0.06 + 5.67E-11*0.03)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.
<G49400c> LTMB       + 0H     = CRES0L           + 2 LCARB0N    : {%TrGAro} 0.141E-11; {&2419} // Same products as for toluene . Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (3.27E-11*0.03 + 3.25E-11*0.03 + 5.67E-11*.04)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.
<G49400d> LTMB       + 0H     = TLBIPER02 +  H02 + 2 LCARB0N    : {%TrGAro} 2.917E-11; {&2419} // Same products as for toluene . Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene
product is produced with a rate constant equal to (3.27E-11*0.70 + 3.25E-11*0.61 + 5.67E-11*0.79)/3, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.
<G49401>  LTMB       + N03    = C6H5CH202 + HN03 + 2 LCARB0N    : {%TrGAro} 1.52E-15;  {&2419} // Same products as for toluene. The rate constant is the average of m, p, o k=(1.90+1.80+0.88)E-15/3=1.52E-15
.
<G40200>  APINENE + 0H          = .75 LAPINAB02 + .15 MENTHEN6ONE + .15 H02 + .10 R006R102 : {%TrGTer} 1.2E-11*EXP(440./TEMP); {&1759} // Products from \citet{3017}. LAPINAB02 = .65 APINA02 + .35 APINB02
<G40201a> LAPINAB02 + N0        = PINAL + H02 + N02               : {%TrGTer} KR02N0*(1.-(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair))); {&2419, 3031}
<G40201b> LAPINAB02 + N0        = LAPINABN03                      : {%TrGTer} KR02N0*(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair)); {&2419, 3031}
<G40202a> LAPINAB02 + H02       = LAPINAB00H                      : {%TrGTer} KR02H02(10)*(1.-rchohch2o2_oh); {&2419, 3031}
<G40202b> LAPINAB02 + H02       = PINAL + H02 + 0H                : {%TrGTer} KR02H02(10)*rchohch2o2_oh; {&2419, 3031}
<G40203>  LAPINAB02             = PINAL + H02                     : {%TrGTer} R02*(0.65*k1_R02t0R02+.35*k1_R02s0R02); {&2419} // Weighted average for isomers A and B, \code{k = 0.33*9.20E-14+0.67*8.80E-
13}.
<G40204>  LAPINAB00H + 0H       = .35 LAPINAB02 + .65 C96C03      : {%TrGTer} 2.77E-11; {&2419} // Weighted average for isomers A and B, \code{k = 0.35*1.83E-11+0.65*3.28E-11}.
<G40205>  LAPINABN03 + 0H       = .35 PINAL + .65 C96C03 + N02    : {%TrGTer} 4.29E-12; {&2419} // Weighted average for isomers A and B, \code{k = 0.35*5.50E-12+0.65*3.64E-12}.
<G40206>  MENTHEN6ONE + 0H      = 0HMENTHEN6ONE02                 : {%TrGTer} 6.46E-11; {&3017} // SAR-estimated rate constant, \code{(kads+kadt)*acoch3 = 6.46E-11} where \code{kads = 3.0E-11}, \code{kadt
= 5.5E-11}, \code{acoch3 = 0.76}
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<G40207>  OHMENTHEN6ONE02 + NO  = OH2MENTHEN6ONE + H02 + N02       : {%TrGTer} KR02NO; {&3017} // \alkylnitrateneglected
<G40208>  OHMENTHEN6ONE02 + H02 = OH2MENTHEN6ONE                   : {%TrGTer} KR02H02(1D); {&3017}
<G40209>  OHMENTHEN6ONE02       = OH2MENTHEN6ONE + H02             : {%TrGTer} k1_R02t0R02; {&3017}
<G40210>  OH2MENTHEN6ONE + OH   = 1D LCARB0N                       : {%TrGTer} 1E-11; {&3017}
<G40211>  PINAL + OH            = .772 C96C03 +  .228 PINAL02      : {%TrGTer} 5.2E-12*EXP(6DD./TEMP); {&1745} // Products from \citet{2419}.
<G40212>  PINAL + N03           = C96C03 + HN03                    : {%TrGTer} 2.0E-14; {&1745} // Products from \citet{2419}.
<G40213a> C96C03                = C96O2 + CO2                      : {%TrGTer} k1_R02RC03*0.9; {&2419}
<G40213b> C96C03                = PIN0NIC                          : {%TrGTer} k1_R02RC03*0.1; {&2419}
<G40214a> C96C03 + H02          = PERPIN0NIC                       : {%TrGTer} KAPH02*rco3_ooh; {&2419}
<G40214b> C96C03 + H02          = PIN0NIC + 03                     : {%TrGTer} KAPH02*rco3_o3; {&2419}
<G40214c> C96C03 + H02          = C96O2 + OH + CO2                 : {%TrGTer} KAPH02*rco3_oh; {&2419}
<G40215>  C96C03 + NO2          = C10PAN2                          : {%TrGTer} k_CH3C03_NO2; {&2419}
<G40216>  C96C03 + NO           = C96O2 + NO2 + CO2                : {%TrGTer} KAPNO; {&2419}
<G40217>  C96C03 + N03          = C96O2 + NO2 + CO2                : {%TrGTer} KR02N03*1.6D; {&2419}
<G40218>  C10PAN2               = C96C03 + NO2                     : {%TrGTer} k_PAN_M; {&2419}
<G40219>  C10PAN2 + OH          = N0RPINAL + CO + NO2              : {%TrGTer} 3.6BE-12; {&2419}
<G40220>  PIN0NIC + OH          = C96O2 + CO2                      : {%TrGTer} 6.65E-12; {&2419}
<G40221>  PERPIN0NIC + OH       = C96C03                           : {%TrGTer} 9.73E-12; {&2419}
<G40222>  PINAL02 + H02         = PINAL00H                         : {%TrGTer} KR02H02(1D); {&2419}
<G40223a> PINAL02 + NO          = C10O2 + NO2                      : {%TrGTer} KR02NO*(1.-alpha_AN(12,3,0,1,0,temp,cair)); {&2419, 3031}
<G40223b> PINAL02 + NO          = PINALN03                         : {%TrGTer} KR02NO*alpha_AN(12,3,0,1,0,temp,cair); {&2419, 3031}
<G40224>  PINAL02               = C10O2                            : {%TrGTer} k1_R02tR02; {&2419}
<G40225>  PINAL00H + OH         = PINAL02                          : {%TrGTer} 2.75E-11; {&2419}
<G40226>  PINALN03 + OH         = C0235C6CH0 + CH3C0CH3 + NO2      : {%TrGTer} 2.25E-11; {&2419}
<G40227>  C10O2 + H02           = C10O00H                          : {%TrGTer} KR02H02(1D); {&2419}
<G40228a> C10O2 + NO            = C7I6O2 + CH3C0CH3 + NO2          : {%TrGTer} KR02NO*0.875*(1.-alpha_AN(13,3,0,0,0,temp,cair)); {&2419, 3031}
<G40228b> C10O2 + NO            = C10I6N03                         : {%TrGTer} KR02NO*0.875*alpha_AN(13,3,0,0,0,temp,cair); {&2419, 3031}
<G40229>  C10O2                 = C7I6O2 + CH3C0CH3                : {%TrGTer} k1_R02tR02; {&2419}
<G40230>  C10O00H + OH          = C10O2                            : {%TrGTer} 8.01E-11; {&2419}
<G40231>  C10I6N03 + OH         = C0235C6CH0 + CH3C0CH3 + NO2      : {%TrGTer} 7.03E-11; {&2419}
<G40232>  APINENE + 03          = .09 APINB00 + .08 PIN0NIC + .77 OH + .33 N0RPINAL + .33 CO + .33 H02 + .06 APINA00 + .44 C10902 : {%TrGTer} 8.05E-16*EXP(-640./TEMP); {&1745} // Products from \citet{3028}.
<G40233>  APINA00               = PINAL + H202                     : {%TrGTer} 1.00E-17*c(ind_H20); {&2419}
<G40234>  APINA00 + CO          = PINAL + CO2                      : {%TrGTer} 1.20E-15; {&2419}
<G40235>  APINA00 + NO          = PINAL + NO2                      : {%TrGTer} 1.00E-14; {&2419}
<G40236>  APINA00 + NO2         = PINAL + NO3                      : {%TrGTer} 1.00E-15; {&2419}
<G40237a> APINB00               = PIN0NIC                          : {%TrGTer} 1.00E-17*c(ind_H20)*(0.08+0.15); {&2419}
<G40237b> APINB00               = PINAL + H202                     : {%TrGTer} 1.00E-17*c(ind_H20)*0.77; {&2419}
<G40238>  APINB00 + CO          = PINAL + CO2                      : {%TrGTer} 1.20E-15; {&2419}
<G40239>  APINB00 + NO          = PINAL + NO2                      : {%TrGTer} 1.00E-14; {&2419}
<G40240>  APINB00 + NO2         = PINAL + NO3                      : {%TrGTer} 1.00E-15; {&2419}
<G40241>  C10902                = C89CO3 + HCH0                    : {%TrGTer} k1_R02p0R02; {&2419}
<G40242>  C10902 + NO           = C89CO3 + HCH0 + NO2              : {%TrGTer} KR02NO; {&2419} // \alkylnitrateneglected
<G40243a> C10902 + H02          = C10900H                          : {%TrGTer} KR02H02(1D)*rcoch2o2_ooh; {&2419, 3031}
<G40243b> C10902 + H02          = C89CO3 + HCH0 + OH               : {%TrGTer} KR02H02(1D)*rcoch2o2_oh; {&2419, 3031}
<G40244>  C10900H + OH          = C109C0 + OH                      : {%TrGTer} 5.47E-11; {&2419}
<G40245>  C109C0 + OH           = C89CO3 + CO                      : {%TrGTer} 5.47E-11; {&2419}
<G40246>  APINENE + N03         = LNAPINAB02                       : {%TrGTer} 1.2E-12*EXP(490./temp); {&1745} // Products from \citet{2419}.
<G40247>  LNAPINAB02            = PINAL + NO2                      : {%TrGTer} (0.65*k1_R02tR02 + 0.35*k1_R02sR02); {&2419}
<G40248>  LNAPINAB02 + NO       = PINAL + NO2 + NO2                : {%TrGTer} KR02NO; {&2419} // \alkylnitrateneglected
<G40249>  LNAPINAB02 + H02      = LNAPINAB00H                      : {%TrGTer} KR02H02(1D); {&2419}
<G40250>  LNAPINAB02 + N03      = PINAL + NO2 + NO2                : {%TrGTer} KR02N03; {&2419}
<G40251>  LNAPINAB00H + OH      = LNAPINAB02                       : {%TrGTer} (.65*6.87E-12+.35*1.23E-11); {&2419}
<G40252a> BPINENE + OH          = BPINA02                          : {%TrGTer} 1.47E-11*EXP(467./TEMP)*(0.8326*0.3+0.068)/(0.8326+0.068); {&3029} // Products from \citet{3019}.
<G40252b> BPINENE + OH          = R006R102                         : {%TrGTer} 1.47E-11*EXP(467./TEMP)*0.8326*0.7/(0.8326+0.068); {&3029} // Products from \citet{3019}.
<G40253a> BPINA02 + H02         = BPINA00H                         : {%TrGTer} KR02H02(1D)*rcoch2o2_ooh; {&2419, 3031}
<G40253b> BPINA02 + H02         = N0PIN0NE + HCH0 + H02 + OH       : {%TrGTer} KR02H02(1D)*rcoch2o2_oh; {&2419, 3031}
<G40254a> BPINA02 + NO          = N0PIN0NE + HCH0 + H02 + NO2      : {%TrGTer} KR02NO*(1.-alpha_AN(11,3,0,0,0,temp,cair)); {&2419, 3031}
<G40254b> BPINA02 + NO          = BPINAN03                         : {%TrGTer} KR02NO*alpha_AN(11,3,0,0,0,temp,cair); {&2419, 3031}
<G40255>  BPINA02               = N0PIN0NE + HCH0 + H02            : {%TrGTer} k1_R02t0R02; {&2419}
<G40256>  BPINA00H + OH         = BPINA02                          : {%TrGTer} 1.33E-11; {&2419}
<G40257>  BPINAN03 + OH         = N0PIN0NE + HCH0 + NO2            : {%TrGTer} 4.70E-12; {&2419}
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<G40258a> R00bR102 + N0          = R00bR302 + CH3C0CH3 + N02        : {%TrGTer} KR02N0*(1.-alpha_AN(13,3,0,0,0,temp,cair)); {&3019}
<G40258b> R00bR102 + N0          = R00bR1N03                        : {%TrGTer} KR02N0*alpha_AN(13,3,0,0,0,temp,cair); {&3019}
<G40259>  R00bR102 + H02         = 1D LCARB0N                       : {%TrGTer} KR02H02(1D); {&3019} // R00bR100H is produced but no sink for it.
<G40260>  R00bR102               = R00bR302 + CH3C0CH3              : {%TrGTer} k1_R02t0R02; {&3019}
<G40261a> R0bR102 + N0           = R0bR302 + N02                    : {%TrGTer} KR02N0*(1.-alpha_AN(12,3,0,0,0,temp,cair)); {&3019}
<G40261b> R0bR102 + N0           = R0bR1N03                         : {%TrGTer} KR02N0*alpha_AN(12,3,0,0,0,temp,cair); {&3019}
<G40262>  R0bR102 + H02          = 1D LCARB0N                       : {%TrGTer} KR02H02(1D); {&3019} // R0bR100H is produced but no sink for it.
<G40263>  R0bR102                = R0bR302                          : {%TrGTer} k1_R02s0R02; {&3019}
<G40264a> R0bR302 + N0           = 9 LCARB0N + HCH0 + H02 + N02     : {%TrGTer} KR02N0*(1.-alpha_AN(12,3,0,0,0,temp,cair)); {&3019}
<G40264b> R0bR302 + N0           = 1D LCARB0N + LNITR0GEN           : {%TrGTer} KR02N0*alpha_AN(12,3,0,0,0,temp,cair); {&3019}
<G40265>  R0bR302 + H02          = 1D LCARB0N                       : {%TrGTer} KR02H02(1D); {&3019}
<G40266>  R0bR302                = 9 LCARB0N + HCH0 + H02           : {%TrGTer} k1_R02sR02; {&3019} // Rate constant modified according to MCM protocol.
<G40267a> BPINENE + 03           = N0PIN0NE + .63 C0 + .37 CH200 + .16 0H + .16 H02 : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.051/(1.-.027); {&1745} // Products from \citet{3018}.
<G40267b> BPINENE + 03           = N0PIN00 + C02                    : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.368/(1.-.027); {&3018, 1745}
<G40267c> BPINENE + 03           = N0PIND02 + C02 + 0H              : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.283/(1.-.027); {&3018, 1745}
<G40267d> BPINENE + 03           = C8BC + 2 C02                     : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*(.104+.167)/(1.-.027); {&3018, 1745}
<G40268>  BPINENE + N03          = LNBPINAB02                       : {%TrGTer} 2.51E-12; {&1745} // Products from \citet{2419}.
<G40269>  LNBPINAB02 + H02       = LNBPINAB00H                      : {%TrGTer} KR02H02(1D); {&2419}
<G40270>  LNBPINAB02 + N0        = N0PIN0NE + HCH0 + N02 + N02      : {%TrGTer} KR02N0; {&2419} // Alkyl nitrate neglected.
<G40271>  LNBPINAB02 + N03       = N0PIN0NE + HCH0 + N02 + N02      : {%TrGTer} KR02N03; {&2419}
<G40272a> LNBPINAB02             = N0PIN0NE + HCH0 + N02            : {%TrGTer} k1_R02tR02*0.7; {&2419}
<G40272b> LNBPINAB02             = BPINAN03                         : {%TrGTer} k1_R02tR02*0.3; {&2419}
<G40273>  LNBPINAB00H + 0H       = LNBPINAB02                       : {%TrGTer} 9.58E-12; {&2419}
<G40274>  R00bR1N03 + 0H         = R00bR302 + CH3C0CH3 + N02        : {%TrGTer} 9.16E-13; {&3019, 3029} // As for R0bR1N03 in G40285.
<G40275>  R0bR1N03 + 0H          = 9 LCARB0N + HCH0 + H02 + N02     : {%TrGTer} 9.16E-13; {&3019, 3029}
<G40276>  PINEN0L + 0H           = HC00H + 0H + N0RPINAL            : {%TrGTer} k_CH2CH0H_0H_HC00H; {&3031, 3179} // \onlythischannel
<G40277>  PINEN0L + HC00H        = PINAL + HC00H                    : {%TrGTer} k_CH2CH0H_HC00H; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G40278>  PINAL  + HC00H         = PINEN0L + HC00H                  : {%TrGTer} k_ALD_HC00H; {&3031, 3162} // Theoretical keto-enol tautomerization catalyzed by formic acid \citep{2040}.
<G40279a> CARENE    + 0H  = LAPINAB02                       : {%TrG} 8.7E-11*(.50+.25); {&3152, 3031}
<G40279b> CARENE    + 0H  = MENTHEN6ONE + H02               : {%TrG} 8.7E-11*.25*.60; {&3152, 3031}
<G40279c> CARENE    + 0H  = R006R102                        : {%TrG} 8.7E-11*.25*.40; {&3152, 3031}
<G40280a> CARENE    + 03  = APINB00                         : {%TrG} 2.E-16*.50*.18; {&3152, 3031}
<G40280b> CARENE    + 03  = PIN0NIC                         : {%TrG} 2.E-16*.50*.16; {&3152, 3031}
<G40280c> CARENE    + 03  = 0H + N0RPINAL + C0 + H02        : {%TrG} 2.E-16*.50*.66; {&3152, 3031}
<G40280d> CARENE    + 03  = APINA00                         : {%TrG} 2.E-16*.50*.12; {&3152, 3031}
<G40280e> CARENE    + 03  = 0H + C10902                     : {%TrG} 2.E-16*.50*(.22+.66); {&3152, 3031}
<G40281>  CARENE    + N03 = LNAPINAB02                      : {%TrG} 9.5E-12; {&3152, 3031}
<G40282a> SABINENE  + 0H  = BPINA02                         : {%TrGTer} 1.47E-11*EXP(467./TEMP)*(0.8326*0.3+0.068)/(0.8326+0.068); {&3029} // Products from \citet{3019}.
<G40282b> SABINENE  + 0H  = R006R102                        : {%TrGTer} 1.47E-11*EXP(467./TEMP)*0.8326*0.7/(0.8326+0.068); {&3019, 3029} // Products from \citet{3019}.
<G40283a> SABINENE  + 03  = N0PIN0NE + .63 C0 + .37 H0CH200H + .16 0H + .16 H02 : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.051/(1.-.027); {&1745} // Products from \citet{3018}.
<G40283b> SABINENE  + 03  = N0PIN00 + C02                    : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.368/(1.-.027); {&3018, 1745}
<G40283c> SABINENE  + 03  = N0PIND02 + C02 + 0H              : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.283/(1.-.027); {&3018, 1745}
<G40283d> SABINENE  + 03  = C8BC + 2 C02                     : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*(.104+.167)/(1.-.027); {&3018, 1745}
<G40284>  SABINENE  + N03 = LNBPINAB02                       : {%TrGTer} 2.51E-12; {&1745} // Products from \citet{2419}.
<G40285a> CAMPHENE  + 0H  = BPINA02                          : {%TrGTer} 1.47E-11*EXP(467./TEMP)*(0.8326*0.3+0.068)/(0.8326+0.068); {&3029} // Products from \citet{3019}.
<G40285b> CAMPHENE  + 0H  = R006R102                         : {%TrGTer} 1.47E-11*EXP(467./TEMP)*0.8326*0.7/(0.8326+0.068); {&3019, 3029} // Products from \citet{3019}.
<G40286a> CAMPHENE  + 03  = N0PIN0NE + .63 C0 + .37 H0CH200H + .16 0H + .16 H02 : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.051/(1.-.027); {&1745} // Products from \citet{3018}.
<G40286b> CAMPHENE  + 03  = N0PIN00 + C02                    : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.368/(1.-.027); {&3018, 1745}
<G40286c> CAMPHENE  + 03  = N0PIND02 + C02 + 0H              : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*.283/(1.-.027); {&3018, 1745}
<G40286d> CAMPHENE  + 03  = C8BC + 2 C02                     : {%TrGTer} 1.35E-15*EXP(-1270./TEMP)*(.104+.167)/(1.-.027); {&3018, 1745}
<G40287>  CAMPHENE  + N03 = LNBPINAB02                       : {%TrGTer} 2.51E-12; {&1745} // Products from \citet{2419}.
<G40400> LHAR0M + 0H  = .14 TLEP0XMUC + .03 C6H5CH202 + .04 CRES0L + .79 TLBIPER02 + .18 H02 + 4 LCARB0N : {%TrGAro} 5.67E-11; {&2419} // DIET35T0L(from MCM) as representative of higher aromatics
<G40401> LHAR0M + N03 = C6H5CH202 + HN03 + 4 LCARB0N                                                    : {%TrGAro} 2.60E-15; {&2419} // Same products as for toluene.
{<G5nnn> ---------------------------- F ----------------------}{@\myhline}
{<G6nnn> ---------------------------- Cl ---------------------}{@\myhline}
<G61D0>  Cl + 03         = ClO + 02    : {%UpStTrG} 2.8E-11*EXP(-250./temp); {&1845}
<G61D1>  ClO + 03P       = Cl + 02     : {%UpStG}   2.5E-11*EXP(110./temp); {&1845}
<G61D2a> ClO + ClO       = Cl2 + 02    : {%StTrG}   1.0E-12*EXP(-1590./temp); {&1845}
<G61D2b> ClO + ClO       = 2 Cl + 02   : {%StTrG}   3.0E-11*EXP(-2450./temp); {&1845}
<G61D2c> ClO + ClO       = Cl + OClO   : {%StTrG}   3.5E-13*EXP(-1370./temp); {&1845}
<G61D2d> ClO + ClO {+M}  = Cl2O2       : {%StTrG}   k_ClO_ClO; {&1845}
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<G6103>  C1202 {+M}      = C10 + C10   : {%StTrG}   k_C10_C10/(1.72E-27*EXP(8649./temp)); {&1845, 2626} // The rate coefficient is defined as backward reaction divided by equilibrium constant.
<G6200>  C1 + H2         = HC1 + H     : {%StG}     3.9E-11*EXP(-2310./temp); {&1845}
<G6201a> C1 + H02        = HC1 + 02    : {%StG}     4.4E-11-7.5E-11*EXP(-620./temp); {&1845}
<G6201b> C1 + H02        = C10 + 0H    : {%StG}     7.5E-11*EXP(-620./temp); {&1845}
<G6202>  C1 + H202       = HC1 + H02   : {%StTrG}   1.1E-11*EXP(-980./temp); {&1845}
<G6203>  C10 + 0H        = .94 C1 + .94 H02 + .06 HC1 + .06 02 : {%StG} 7.3E-12*EXP(300./temp); {&1845}
<G6204>  C10 + H02       = H0C1 + 02   : {%StTrG}   2.2E-12*EXP(340./temp); {&1845} // At low temperatures, there may be a minor reaction channel leading to \kpp{03}+\kpp{HC1}. See \citet{1626} for details.
It is neglected here.
<G6205>  HC1 + 0H        = C1  + H20   : {%StTrG}   1.7E-12*EXP(-230./temp); {&1845}
<G6206>  H0C1 + 0H       = C10 + H20   : {%StG}     3.0E-12*EXP(-500./temp); {&2626}
<G6300>  C10   + N0       = N02 + C1   : {%UpStTrG} 6.2E-12*EXP(295./temp); {&1845}
<G6301>  C10   + N02 {+M} = C1N03      : {%StTrG}   k_3rd_iupac(temp,cair,1.6E-31,3.4,7.E-11,0.,0.4); {&1845}
<G6302>  C1N03           = C10 + N02   : {%TrG}     6.918E-7*EXP(-10909./temp)*cair; {&1059} {10^(+/-0.15)}
<G6303>  C1N03 + 03P     = C10 + N03   : {%StG}     4.5E-12*EXP(-900./temp); {&1845}
<G6304>  C1N03 + C1      = C12 + N03   : {%StTrG}   6.2E-12*EXP(145./temp); {&1845}
<G6400>  C1      + CH4    = HC1 + CH3         : {%StTrG} 6.6E-12*EXP(-1240./temp); {&1759}
<G6401>  C1      + HCH0   = HC1 + C0 + H02    : {%StTrG} 8.1E-11*EXP(-34./temp); {&1759}
<G6402>  C1      + CH300H = HCH0 + HC1 + 0H   : {%StTrG} 5.9E-11; {&1759} // The initial products are probably \chem{HC1} and \chem{CH_200H} \citep{1759}. It is assumed that \chem{CH_200H} dissociates into
\chem{HCH0} and \chem{0H}.
<G6403>  C10     + CH302  = H02 + C1 + HCH0   : {%StTrG} 3.3E-12*EXP(-115./temp); {&2626}
<G6404>  CC14    + 01D    = LCARB0N + C10 + 3 C1 {+...} : {%StG} 3.3E-10; {&2626}
<G6405>  CH3C1   + 01D    = LCARB0N + 0H + C1 {+...} : {%StG} 1.65E-10; // Average of reactions with \chem{CH_3Br} and \chem{CH_3F} from \citet{1945} (B.\ Steil, pers.\ comm.).
<G6406>  CH3C1   + 0H     = LCARB0N + H20 + C1 {+...} : {%StG} 2.4E-12*EXP(-1250./temp); {&2626}
<G6407>  CH3CC13 + 01D    = 2 LCARB0N + 0H + 3 C1 {+...} : {%StG} 3.E-10; // Rough extrapolation from reactions with \chem{CH_3CF_3}, \chem{CH_3CC1F_2}, and \chem{CH_3CC1_2F} from \citet{1945}.
<G6408>  CH3CC13 + 0H     = 2 LCARB0N + H20 + 3 C1 {+...} : {%StTrG} 1.64E-12*EXP(-1520./temp); {&2626}
<G6409>  C1 + C2H4 {+02}  = H0CH2CH202 + HC1  : {%TrG} k_3rd_iupac(temp,cair,1.85E-29,3.3,6.0E-10,0.0,0.4); {&1759} // It is assumed that the reaction liberates all \kpp{Cl} atoms in the form of \kpp{HCl}.
<G6410>  C1      + CH3CH0 = HC1 + CH3C0      : {%TrG} 8.0e-11; {&1759}
<G6411>  C2H2    + C1     = LCARB0N + CH3 + HC1       : {%TrG} k_3rd_iupac(temp,cair,6.1e-30,3.0,2.0e-10,0.,0.6); {&1759}
<G6412>  C2H6    + C1     = C2H502 + HC1       : {%TrG} 8.3E-11*EXP(-100./temp); {&1759}
<G6413>  C1      + CH3N03 = HC1 + HCH0 + N02   : {%StTrG} 1.3E-11*EXP(-1200./temp); {&2626}
<G6414>  C1      + CH30N0 = HC1 + HCH0 + N0    : {%StTrG} 2.1E-12; {&3063}
<G6415>  C1      + CH302  = .5 C10 + .5 CH30 + .5 HC1 + .5 CH200 : {%StTrG} 1.6E-10; {&2626}
<G6416>  C1      + CH3CN  = NCCH202 + HC1      : {%TrG} 1.6E-11*EXP(-2104./temp); {&3211, 3212, 3031}
<G6500>  CF2C12  + 01D    = LCARB0N + 2 LFLU0RINE + C10 + C1 {+...}   : {%StG} 1.4E-10; {&2626}
<G6501>  CFC13   + 01D    = LCARB0N + LFLU0RINE + C10 + 2 C1 {+...} : {%StG} 2.3E-10; {&2626}
{<G7nnn> ---------------------------- Br ----------------------}{@\myhline}
<G7100>  Br   + 03       = Br0 + 02       : {%StTrG}   1.7E-11*EXP(-800./temp); {&1845}
<G7101>  Br0  + 03P      = Br + 02        : {%StG}     1.9E-11*EXP(230./temp); {&1845}
<G7102a> Br0  + Br0      = 2 Br + 02      : {%StTrG}   2.7E-12; {&1845}
<G7102b> Br0  + Br0      = Br2 + 02       : {%StTrG}   2.9E-14*EXP(840./temp); {&1845}
<G7200>  Br   + H02      = HBr + 02       : {%StTrG}   7.7E-12*EXP(-450./temp); {&1845}
<G7201>  Br0  + H02      = H0Br + 02      : {%StTrG}   4.5E-12*EXP(500./temp); {&1845}
<G7202>  HBr  + 0H       = Br  + H20      : {%StTrG}   6.7E-12*EXP(155./temp); {&1845}
<G7203>  H0Br + 03P      = 0H  + Br0      : {%StG}     1.2E-10*EXP(-430./temp); {&1845}
<G7204>  Br2  + 0H       = H0Br + Br      : {%StTrG}   2.0E-11*EXP(240./temp); {&1845}
<G7300>  Br   + BrN03    = Br2 + N03      : {%TrG}    4.9E-11{4.9+/-1.5}; {&1054}
<G7301>  Br0  + N0       = Br  + N02      : {%StTrG}  8.7E-12*EXP(260./temp); {&1845}
<G7302>  Br0  + N02 {+M} = BrN03          : {%StTrG}  k_Br0_N02; {&1845} // The rate coefficient is: \code{k_Br0_N02} = \code{k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)}.
<G7303>  BrN03           = Br0 + N02      : {%TrG}    k_Br0_N02/(5.44E-9*EXP(14192./temp)*1.E6*R_gas*temp/(atm2Pa*N_A)); {&1054, 1845} // The rate coefficient is defined as backward reaction \citep{1845}
divided by equilibrium constant \citep{1054}.
<G7400>  Br   + HCH0     = HBr + C0 + H02    : {%StTrG} 7.7E-12*EXP(-580./temp); {&1759}
<G7401>  Br   + CH300H   = CH302 + HBr       : {%TrG} 2.6E-12{10^(+/-0.3)}*EXP(-1600./temp); {&416}
<G7402>  Br0  + CH302    = H0Br + CH200      : {%TrG} 2.42E-14*EXP(1617./temp); {&3205}
<G7403>  CH3Br + 0H      = LCARB0N + H20 + Br {+...} : {%StTrG} 2.35E-12*EXP(-1300./temp); {&2626}
<G7404>  Br + C2H4 {+02} = H0CH2CH202 + HBr : {%TrG} 2.8E-13*EXP(224./temp)/(1.+1.13E24*EXP(-3200./temp)/C(ind_02)); {&1759} // It is assumed that the reaction liberates all \kpp{Br} atoms in the form of
\kpp{HBr}.
<G7405>  Br   + CH3CH0   = HBr + CH3C0     : {%TrG} 1.8e-11*EXP(-460./temp); {&1759}
<G7406>  Br   + C2H2     = LCARB0N + CH302 + HBr      : {%TrG} 6.35e-15*EXP(440./temp); {&1759}
<G7407>  CHBr3  + 0H     = LCARB0N + H20 + 3 Br {+...}: {%TrG} 1.35E-12*EXP(-600./temp); {&2626} // It is assumed that the reaction liberates all \kpp{Br} atoms. The fate of the carbon atom is currently not
considered.
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<G7408>  CH2Br2 + OH     = LCARBON + H2O + 2 Br {+...}: {%TrG} 2.0E-12*EXP(-840./temp); {&2626} // It is assumed that the reaction liberates all \kpp{Br} atoms. The fate of the carbon atom is currently not considered.
<G7600>  Br   + BrCl     = Br2  + Cl        : {%TrG}   3.32E-15; {&2517}
<G7601>  Br   + Cl2      = BrCl + Cl        : {%TrG}   1.10E-15{1.1+/-0.4}; {&2518}
<G7602>  Br2  + Cl       = BrCl + Br        : {%TrG}   2.3E-10{2.3+/-0.4}*EXP(135./temp); {&2519}
<G7603a> BrO  + ClO      = Br   + OClO      : {%StTrG} 1.6E-12*EXP(430./temp); {&1845}
<G7603b> BrO  + ClO      = Br   + Cl + O2   : {%StTrG} 2.9E-12*EXP(220./temp); {&1845}
<G7603c> BrO  + ClO      = BrCl + O2        : {%StTrG} 5.8E-13*EXP(170./temp); {&1845}
<G7604>  BrCl + Cl       = Br   + Cl2       : {%TrG}   1.45E-11{1.45+/-0.2}; {&2520}
<G7605>  CHCl2Br + OH    = LCARBON + 2 LCHLORINE + H2O + Br   {+CH3O2} : {%TrG} 2.0E-12*EXP(-840./temp); // Same value as for G7408: \kpp{CH2Br2}+\kpp{OH} assumed. It is assumed that the reaction liberates all \kpp{Br} atoms but not \kpp{Cl}. The fate of the carbon atom is currently not considered.
<G7606>  CHClBr2 + OH    = LCARBON + LCHLORINE + H2O + 2 Br {+CH3O2} : {%TrG} 2.0E-12*EXP(-840./temp); // Same value as for G7408: \kpp{CH2Br2}+\kpp{OH} assumed. It is assumed that the reaction liberates all \kpp{Br} atoms but not \kpp{Cl}. The fate of the carbon atom is currently not considered.
<G7607>  CH2ClBr + OH    = LCARBON + LCHLORINE + H2O + Br   {+CH3O2} : {%TrG} 2.4E-12*EXP(-920./temp); {&2626} // It is assumed that the reaction liberates all \kpp{Br} atoms but not \kpp{Cl}. The fate of the carbon atom is currently not considered.
{<G8nnn> ---------------------------- I ------------------------}{@\myhline}
<G8100>  I     + O3    = IO + O2           : {%TrG} 2.1E-11*EXP(-830./temp); {&1845}
<G8102>  OIO   + OIO   = IPART             : {%TrG} 5.E-11; {&1456} // It is assumed that the reaction produces new particles.
<G8103>  IO    + IO    = .38 OIO + 1.62 I + .62 O2 : {%TrG} 5.4E-11*EXP(180./temp); {&1845} // The yield of 38~\unit{\%} \chem{OIO} is from \citet{1845}. It is assumed here that the remaining 62~\unit{\%} produce 2 \chem{I} + \chem{O_2}.
<G8200>  I     + HO2   = HI  + O2          : {%TrG} 1.5E-11*EXP(-1090./temp); {&1845}
<G8201>  IO    + HO2   = HOI + O2          : {%TrG} 1.4E-11*EXP(540./temp); {&1845}
<G8202>  HI    + OH    = I   + H2O         : {%TrG} 1.6E-11*EXP(440./temp); {&1845}
<G8203>  OIO   + OH    = HIO3              : {%TrG} 2.2E-10*EXP(243./temp); {&1788}
<G8204>  I2    + OH    = HOI + I           : {%TrG} 2.1E-10; {&1845}
<G8300>  I + NO2 {+M}  = INO2              : {%TrG} k_I_NO2; {&1845} // The rate coefficient is: \code{k_I_NO2} = \code{k_3rd_iupac(temp,cair,3.E-31,1.,6.6E-11,0.,0.63)}.
<G8301>  I     + NO3   = IO + NO2          : {%TrG} 1.E-10{1.0+/-0.3}; {&2244}
<G8302>  IO    + NO    = I  + NO2          : {%TrG} 7.15E-12*EXP(300./temp); {&1845}
<G8303>  IO + NO2 {+M} = INO3              : {%TrG} k_3rd_iupac(temp,cair,7.7E-31,5.,1.6E-11,0.,0.4); {&1845}
<G8304>  OIO   + NO    = NO2 + IO          : {%TrG} 1.1E-12*EXP(542./temp); {&1845}
<G8305>  INO2          = I + NO2           : {%TrG} k_I_NO2/(3.7E-7{10^(+/-0.3)}*EXP(9568./temp)*1.E6*R_gas*temp/(atm2Pa*N_A)); {&1644, 1845} // The rate coefficient is defined as backward reaction \citep{1845} divided by equilibrium constant \citep{1644}.
<G8306>  INO3          = IO + NO2          : {%TrG} 0.; // According to John Plane and John Crowley (pers.\ comm.\ 2007), the rate coefficient of \code{1.1E15*EXP(-12060./temp)} suggested by \citet{1845} is wrong.
<G8307>  I2    + NO3   = I + INO3          : {%TrG} 1.5E-12; {&1845}
<G8308>  IO    + NO3   = OIO + NO2         : {%TrG} 9.E-12{9+/-4}; {&2244}
<G8400>  C3H7I + OH    = 2 LCARBON + CH3O2 + I         : {%TrG} 1.22E-12{1.22+/-0.06}; {&1503}
<G8401>  CH3O2 + IO    = .4 I + .6 OIO + HCHO + HO2 : {%TrG} 2.E-12{2.0+/-1.0}; {&2079, 2089} // The rate coefficient is from \citet{2079}, the yield of \chem{I} atoms is a lower limit given on page 2170 of \citet{2089}.
<G8402>  CH3I + NO3 {+O2} = HNO3 + HCHO + IO : {%TrG} 3.4E-17; {&94} // The products are from \citet{2087}.
<G8600>  IO    + ClO   = .2 ICl + .25 Cl + .55 OClO + .8 I + .45 O2 : {%TrG} 4.7E-12*EXP(280./temp); {&1845} {products: 20% ICl+O2, 25% I+Cl+O2, 55% I+OClO}
<G8700>  I     + BrO   = IO + Br           : {%TrG} 1.2E-11; {&2626}
<G8701>  IO    + BrO   = Br + .8 OIO + .2 I + .2 O2 : {%TrG} 1.5E-11*EXP(510./temp); {&1845} // 80\% \chem{Br} + \chem{OIO} production is from \citet{1845}. The remaining channels are assumed to produce \chem{Br} + \chem{I} + \chem{O_2}.
{<G9nnn> ---------------------------- S ------------------------}{@\myhline}
<G9200a>  SO2    + OH    = SO3 + HO2 : {%StTrGS}   k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0.,0.6); {&2626}
<G9400a> DMS    + OH    = CH3SO2 + HCHO       : {%TrG} 1.13E-11*EXP(-253./temp); {&1610} // For the abstraction path, the assumed reaction sequence (omitting \chem{H_2O} and \chem{O_2} as products) according to \citet{243} is: \begin{eqnarray*} \chem{DMS} + \chem{OH} & \TO & \chem{CH_3SCH_2}\\ \chem{CH_3SCH_2} + \chem{O_2} & \TO & \chem{CH_3SCH_2OO}\\ \chem{CH_3SCH_2OO} + \chem{NO} & \TO & \chem{CH_3SCH_2O} + \chem{NO_2}\\ \chem{CH_3SCH_2O} & \TO & \chem{CH_3S} + \chem{HCHO}\\ \chem{CH_3S} + \chem{O_3} & \TO & \chem{CH_3SO}\\ \chem{CH_3SO} + \chem{O_3} & \TO & \chem{CH_3SO_2}\\ \hline \chem{DMS}+\chem{OH}+\chem{NO}+2\chem{O_3} & \TO & \chem{CH_3SO_2}+\chem{HCHO}+\chem{NO_2} \end{eqnarray*} Neglecting the effect on \chem{O_3} and \chem{NO_x}, the remaining reaction is: $$\chem{DMS} + \chem{OH} + \chem{O_3} \TO \chem{CH_3SO_2} + \chem{HCHO}$$.
<G9400b> DMS    + OH    = DMSO + HO2          : {%TrG} k_DMS_OH; {&1610} // For the addition path, the rate coefficient is: \code{k_DMS_OH} = \code{1.0E-39*EXP(5820./temp)*C(ind_O2)/ (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))}.
<G9401>  DMS    + NO3   = CH3SO2 + HNO3 + HCHO  {-O3}: {%TrG} 1.9E-13*EXP(520./temp); {&1610}
<G9402>  DMSO   + OH    = .6 SO2 +  HCHO + .6 CH3 + .4 HO2 + .4 CH3SO3H : {%TrG} 1.E-10{1.0+/-0.3}; {&746}
<G9403>  CH3SO2         = SO2 + CH3         : {%TrG} 1.8E13*EXP(-8611./temp); {&749}
<G9404>  CH3SO2 + O3    = CH3SO3            : {%TrG} 3.E-13; {&749}
<G9405>  CH3SO3 + HO2   = CH3SO3H           : {%TrG} 5.E-11; {&749}
<G9408>  CH2OO + SO2 {+H2O} = H2SO4 + HCHO  : {%StTrG} k_CH2OO_SO2; {&3041, 3049} // Average of 3.9E-11 and 3.42E-11.
<G9409>  NOPINOO + SO2 = NOPINONE + H2SO4   : {%TrGTer} 7.E-14; {&2419}
<G9410>  APINAOO + SO2 = PINAL + H2SO4      : {%TrGTer} 7.00E-14; {&2419}
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<G9411>  APINB00 + SO2 = PINAL + H2SO4      : {%TrGTer} 7.00E-14; {&2419}
<G9412>  MB000 + SO2   = IBUTAL0H + H2SO4   : {%TrGTer} 7.00E-14; {&2419}
<G9600>  DMS + Cl       = CH3SO2 + HCl + HCHO : {%TrG} 3.3E-10; {&1610}
<G9700>  DMS + Br       = CH3SO2 + HBr + HCHO : {%TrG} 9.E-11{9.0+/-2.9}*EXP(-2386.{2386+/-151}/temp); {&2399}
<G9701>  DMS + BrO      = DMSO + Br           : {%TrG} 4.4E-13{4.4+/-0.66}; {&9332}
<G9800>  DMS + IO       = DMSO + I            : {%TrG} 3.2E-13{3.2+/-1.4}*EXP(-925.{925+/-136}/temp); {&2080}
{<G10nnn> ------------------------------ Hg ------------------------}{@\myhline}
<G10100>  Hg + O3       = HgO + O2            : {%TrG} 3.0E-20{3+/-2}; {&2394}
<G10200>  Hg + OH       = HgO + H             : {%TrG} 3.55E-14{9+/-1.3}*EXP(294.{294+/-16}/temp); {&2252}
<G10201>  Hg + H2O2     = HgO + H2O           : {%TrG} 8.5E-19; {&2248} // Upper limit.
<G10600>  Hg + Cl       = HgCl                : {%TrG} 1.0E-11{1.0+/-0.2}; {&2246}
<G10601>  Hg + Cl2      = HgCl2               : {%TrG} 2.6E-18{2.6+/-0.2}; {&2246}
<G10700>  Hg + Br       = HgBr                : {%TrG} 3.0E-13; {&2282}
<G10701>  HgBr + Br     = HgBr2               : {%TrG} 2.5E-10*(temp/298.)**(-0.57); {&2274}
<G10702>  Hg + Br2      = HgBr2               : {%TrG} 9.0E-17{9+/-2}; {&2246}
<G10703>  Hg + BrO      = HgO + Br            : {%TrG} 1.0E-15; {&2261}{lower limit}
<G10704>  HgBr + BrO    = BrHgOBr             : {%TrG} 3.0E-12; {&2273}
<G10705>  HgCl + BrO    = ClHgOBr             : {%TrG} 3.0E-12; {&2273}
<G10706>  HgBr + Cl     = ClHgBr              : {%TrG} 3.0E-12; {&2273}
<G10707>  HgCl + Br     = ClHgBr              : {%TrG} 3.0E-12; {&2273}
{<J0nnn> ------------------------------ e* ------------------------}{@\myhline}
{<J1nnn> ------------------------------ O ------------------------}{@\myhline}
<J1000a> O2      + hv = O3P + O3P             : {%UpStTrGJ} jx(ip_O2); {&2342}
<J1001a> O3      + hv = O1D + O2              : {%UpStTrGJ} jx(ip_O1D); {&2342}
<J1001b> O3      + hv = O3P + O2              : {%UpStTrGJ} jx(ip_O3P); {&2342}
{<J2nnn> ------------------------------ H ------------------------}{@\myhline}
<J2100a> H2O     + hv = H + OH     : {%UpStGJ}   jx(ip_H2O); {&2342}
<J2101>  H2O2    + hv = 2 OH       : {%UpStTrGJ} jx(ip_H2O2); {&2342}
{<J3nnn> ------------------------------ N ------------------------}{@\myhline}
<J3100>  N2O     + hv = O1D + N2   : {%UpStGJ}    jx(ip_N2O); {&2342}
<J3101>  NO2     + hv = NO + O3P   : {%UpStTrGJ}  jx(ip_NO2); {&2342}
<J3102a> NO      + hv = N + O3P    : {%UpStGJ}    jx(ip_NO); {&2342}
<J3103a> NO3     + hv = NO2 + O3P  : {%UpStTrGJ}  jx(ip_NO2O); {&2342}
<J3103b> NO3     + hv = NO  + O2   : {%UpStTrGJ}  jx(ip_NOO2); {&2342}
<J3104>  N2O5    + hv = NO2 + NO3  : {%StTrGJ}    jx(ip_N2O5); {&2342}
<J3200>  HONO    + hv = NO + OH    : {%TrGJ} jx(ip_HONO); {&2342}
<J3201>  HNO3    + hv = NO2 + OH   : {%StTrGJ} jx(ip_HNO3); {&2342}
<J3202>  HNO4    + hv = .667 NO2 + .667 HO2 + .333 NO3 + .333 OH : {%StTrGJ} jx(ip_HNO4); {&2342}
{<J4nnn> ------------------------------ C ------------------------}{@\myhline}
<J4100>  CH3OOH      + hv = CH3O + OH                 : {%StTrGJ} jx(ip_CH3OOH); {&2342}
<J4100a> HCHO        + hv = H2 + CO                   : {%StTrGJ} jx(ip_COH2); {&2342}
<J4100b> HCHO        + hv = H + CO + HO2              : {%StTrGJ} jx(ip_CHOH); {&2342}
<J4100c> CO2         + hv = CO + O3P                  : {%StGJ}   jx(ip_CO2); {&2342}
<J4100d> CH4         + hv = .42 CH3 + .42 H + .6912 H2 + .0864 HCHO + .0864 O3P + .1584 OH + .1584 HO2 + .2112 CO2 + .1824 CO + .024 H2O + .10 LCARBON : {%StGJ} jx(ip_CH4); {&2342} // \chem{CH_3}- and
\chem{CH_2}-channels are considered only and with their branching ratios being 0.42 and 0.48, respectively \citep{3058}. \chem{CH}-production is neglected. \chem{CH_2} is assumed to react only with O2
yielding 1.44 \chem{H_2} + .18 \chem{HCHO} + .18 \chem{O(^3P)} + .33 \chem{OH} + .33 \chem{HO_2} + .44 \chem{CO_2} + .38 \chem{CO} + .05 \chem{H_2O} as assumed in the WACCM model by J. Orlando (Doug
Kinnison, pers. comm. with D. Taraborrelli).
<J4100e> CH3ONO      + hv = CH3O + NO                 : {%StTrGJ} jx(ip_CH3ONO); {&2342}
<J4100f> CH3NO3      + hv = CH3O + NO2                : {%StTrGJ} jx(ip_CH3NO3); {&2342}
<J4100g> CH3O2NO2    + hv = .667 NO2 + .667 CH3O2 + .333 NO3 + .333 CH3O : {%StTrGJ} jx(ip_CH3O2NO2); {&2342} // product distribution as for HNO4
<J4100h> HOCH2OOH    + hv = HCOOH + OH + HO2          : {%StTrGJ} jx(ip_CH3OOH); {&2342}
<J4100i> CH3O2       + hv = HCHO + OH                 : {%StTrGJ} jx(ip_CH3O2); {&2342}
<J4100j> HCOOH       + hv = CO + HO2 + OH             : {%StTrGJ} jx(ip_HCOOH); {&2342}
<J4101>  HOCH2O2NO2  + hv = .667 NO2 + .667 HOCH2O2 + .333 NO3 + .333 HCOOH + .333 HO2 : {%StTrGJ} jx(ip_CH3O2NO2); {&2342}
<J4200>  C2H5OOH     + hv = CH3CHO + HO2 + OH        : {%TrGJ}  jx(ip_CH3OOH); {&1612}
<J4200a> CH3CHO      + hv = CH3 + HO2 + CO           : {%TrGJ}  jx(ip_CH3CHO); {&2342}
<J4200b> CH3CHO      + hv = CH2CHOH                  : {%TrGJ}  jx(ip_CH3CHO2VINY); {&3160}
<J4200c> CH3CO3H     + hv = CH3 + OH  + CO2          : {%TrGJ}  jx(ip_CH3CO3H); {&2342}
<J4200d> PAN         + hv = .7 CH3CO + .7 NO2 + .3 CH3 + .3 CO2 + .3 NO3 : {%TrGJ} jx(ip_PAN); {&2342, 2626}
<J4200e> HOCH2CHO    + hv = HCHO + 2 HO2 + CO        : {%TrGJ}  jx(ip_HOCH2CHO)*0.83; {&2626}
<J4200f> HOCH2CHO    + hv = OH + HCOCH2O2            : {%TrGJ}  jx(ip_HOCH2CHO)*0.07; {&2626}
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<J42005c> HOCH2CHO    + hv = CH3OH + CO              : {%TrGJ}  jx(ip_HOCH2CHO)*0.10; {&2626}
<J42006> HOCH2CO3H   + hv = HCHO + HO2 + OH + CO2    : {%TrGJ}  jx(ip_CH3OOH); {&2419}
<J42007> PHAN        + hv = .7 HOCH2CO + .7 NO2 + .3 HCHO + .3 HO2 + .3 CO2 +.3 NO3  : {%TrGJ} jx(ip_PAN); // It is assumed that J(\kpp{PHAN}) is the same as J(\kpp{PAN}).
<J42008> GLYOX       + hv = 2 CO + 2 HO2          : {%TrGJ} jx(ip_GLYOX); {&2342}
<J42009> HCOCO2H     + hv = 2 HO2 + CO + CO2              : {%TrGJ} jx(ip_MGLYOX); {&2419}
<J42010> HCOCO3H     + hv = HO2 + CO + OH + CO2           : {%TrGJ} jx(ip_CH3OOH)+jx(ip_HOCH2CHO); {&2419}
<J42011> HYETHO2H    + hv = HOCH2CH2O + OH                : {%TrGJ} jx(ip_CH3OOH); {&2419}
<J42012> ETHOHNO3    + hv = HO2 + 2 HCHO + NO2            : {%TrGJ} J_IC3H7NO3; {&2419}
<J42013> HOOCH2CO3H  + hv = OH + HCHO + CO2 + OH          : {%TrGJ} 2*jx(ip_CH3OOH); {&3031}
<J42014> HOOCH2CO2H  + hv = OH + HCHO + HO2 + CO2         : {%TrG}  jx(ip_CH3OOH); {&3031}
<J42015> CH2CO       + hv = .4 CO2 + .8 H + .34 CO + .34 OH + .34 HO2 + .16 HCHO + .16 O3P + .1 HCOOH + CO    : {%TrG} J_ketene* 0.36; {&3031}
<J42016> CH3CHOHOOH  + hv = CH3 + HCOOH + OH              : {%TrG}  jx(ip_CH3OOH); {&3031}
<J42017> NO3CH2CHO   + hv = HO2 + CO + HCHO + NO2         : {%TrGJ} (jx(ip_C2H5NO3)+jx(ip_CH3CHO))*(jx(ip_NOA)+1E-10)/(0.59*J_IC3H7NO3+jx(ip_CH3COCH3)+1E-10); {&3031} // Enhancement of J according to
\citet{3168}.
<J42018> HOOCH2CHO   + hv = OH + HCHO + CO + HO2          : {%TrGJ} jx(ip_CH3OOH)+jx(ip_HOCH2CHO); {&3031}
<J42019> C2H5NO3     + hv = CH3CHO + HO2 + NO2            : {%TrGJ} jx(ip_C2H5NO3); {&3031}
<J42020> NO3CH2PAN   + hv = .7 NO3CH2CO3 + .7 NO2 + .3 HCHO + .3 NO2 + .3 CO2 + .3 NO3 : {%TrGJ} jx(ip_PAN); {&3031} // It is assumed that J(\kpp{NO3CH2PAN}) is the same as J(\kpp{PAN}).
<J42021> C2H5O2NO2   + hv = .667 NO2 + .667 C2H5O2 + .333 NO3 + .333 CH3CHO + .333 HO2 : {%StTrGJ} jx(ip_CH3O2NO2); {&3031} // In analogy to what is assumed for \kpp{CH3O2NO2} photolysis as in
\citep{2342}.
<J43000> IC3H7OOH     + hv = CH3COCH3 + HO2 + OH         : {%TrGJ} jx(ip_CH3OOH); {&1612}
<J43001> CH3COCH3     + hv = CH3CO + CH3                 : {%TrGJ} jx(ip_CH3COCH3); {&2342}
<J43002> ACETOL       + hv = .5 CH3CO + .5 HCHO + .5 HO2 + .5 HOCH2CO + .5 CH3 : {%TrGJ} J_ACETOL; {&2626} // Following \citet{1584}, we use J(\kpp{ACETOL}) = \code{0.11*jx(ip_CHOH)}. As an additional
factor, the quantum yield of 0.65 is taken from \citet{2510}.
<J43003> MGLYOX       + hv = CH3CO + CO + HO2            : {%TrGJ} jx(ip_MGLYOX); {&2342}
<J43004> HYPERACET    + hv = CH3CO + HCHO + OH           : {%TrGJ} jx(ip_CH3OOH)+J_ACETOL; {&2419}
<J43005> HOCH2COCH2OOH + hv = HOCH2CO + HCHO + OH        : {%TrGJ} jx(ip_CH3OOH)+J_ACETOL; {&3031}
<J43006> IC3H7NO3     + hv = CH3COCH3 + NO2 + HO2        : {%TrGJ} J_IC3H7NO3; {&1584} // Following \citet{1584}, we use J(\kpp{IC3H7NO3}) = \code{3.7*jx(ip_PAN)}.
<J43007> NOA          + hv = CH3CO + HCHO + NO2          : {%TrGJ} jx(ip_NOA); {&3146}
<J43009> HYPROPO2H    + hv = CH3CHO + HCHO + HO2 + OH    : {%TrGJ} jx(ip_CH3OOH); {&2419}
<J43010> PR2O2HNO3    + hv = NOA + HO2 + OH              : {%TrGJ} jx(ip_CH3OOH); {&2419}
<J43011> HOCH2COCHO   + hv = HOCH2CO + CO + HO2          : {%TrGJ} jx(ip_MGLYOX); {&2419}
<J43012> ALCOCH2OOH   + hv = HCOCO + HCHO + OH           : {%TrGJ} jx(ip_CH3OOH)+J_ACETOL; {&3031}
<J43013> ALCOCH2OOH   + hv = HOOCH2CO3 + CO + HO2        : {%TrGJ} jx(ip_MGLYOX); {&3031}
<J43014> HCOCH2CHO    + hv = HCOCH2O2 + HO2 + CO         : {%TrGJTer} jx(ip_HOCH2CHO)*2.; {&2419}
<J43015> HCOCH2CO2H   + hv = HCOCH2O2 + CO2 + HO2        : {%TrGJTer} jx(ip_HOCH2CHO); {&2419}
<J43016> HOC2H4CO3H   + hv = HOCH2CH2O2 + CO2 + OH       : {%TrGJTer} jx(ip_CH3OOH); {&2419}
<J43017> C3HCO        + hv = HCOCO + HO2 + CO            : {%TrGJ} 2.*jx(ip_MGLYOX); {&3031}
<J43018> CH3COCO2H    + hv = .32 CH3CHO + .16 CH2CHOH + .54 CO2 + .38 CH3CO + .38 HO2 + .38 CO2 + .07 CH3CO2H + .07 CO + .05 CH3CO + .05 CO + .05 OH : {%TrGJ} JX(IP_CH3COCO2H); {&2626, 3031} // One third
of the acetaldehyde channel is considered to be CH2CHOH according to Hjorth (2002) EUPHORE Report.
<J43019> CH3COCO3H    + hv = CH3CO + OH + CO2            : {%TrG} JX(IP_MGLYOX)+jx(ip_CH3OOH); {&3031}
<J43020> CH3CHCO      + hv = C2H4 + CO                   : {%TrG} J_ketene*0.36*2.; {&3031}
<J43021> PROPOLNO3    + hv = HOCH2CHO + HCHO + HO2 + NO2 : {%TrG} J_IC3H7NO3; {&3031}
<J43022> CH3COCH2O2NO2 + hv = CH3CO + HCHO + NO3         : {%TrG} jx(ip_CH3O2NO2)+jx(ip_CH3COCH3); {&3031}
<J43023> NC3H7OOH     + hv = C2H5CHO + HO2 + OH          : {%TrGJ} jx(ip_CH3OOH); {&1612}
<J43024> NC3H7NO3     + hv = C2H5CHO + NO2 + HO2         : {%TrGJ} 0.59*J_IC3H7NO3; // Assuming J(\kpp{NC3H7NO3}) = 0.59 $\times$ J(\kpp{IC3H7NO3}), consistent with the photolysis rate coefficients used
in the MCM \citep{2419}.
<J43025a> C2H5CHO     + hv = C2H5O2 + HO2 + CO           : {%TrGJ} jx(ip_C2H5CHO2HCO); // Photolysis frequencies very similar to the ones of \kpp{CH3CHO}.
<J43025b> C2H5CHO     + hv = PROPENOL                    : {%TrGJ} jx(ip_C2H5CHO2ENOL); {&3161, 3031} // Photolysis frequencies very similar to the ones of \kpp{CH3CHO}.
<J43026> PPN          + hv = .7 C2H5CO3 + .7 NO2 + .3 C2H5O2 + .3 CO2 + .3 NO3   : {%TrGJ} jx(ip_PAN); {&2342, 2626}
<J43027> C2H5CO3H     + hv = C2H5O2 + CO2 + OH           : {%TrGJ} jx(ip_CH3OOH); {&1612}
<J43028a> HCOCOCH2OOH  + hv = HOOCH2CO3 + CO + HO2       : {%TrGJ} jx(ip_MGLYOX); {&3031}
<J43028b> HCOCOCH2OOH  + hv = HCOCO + HCHO + OH          : {%TrGJ} jx(ip_HOCH2CHO)+jx(ip_CH3OOH); {&3031}
<J43200> HCOCH2CO3H   + hv = HCOCH2O2 + CO2 + OH         : {%TrGJTer} jx(ip_HOCH2CHO)+jx(ip_CH3OOH); {&2419}
<J43400> C3DIALOOH    + hv = GLYOX + CO + HO2 + OH       : {%TrGJAro} jx(ip_HOCH2CHO)*2+jx(ip_CH3OOH); {&2419} // KDEC C3DIALO $\rightarrow$ GLYOX + CO + HO2
<J43401> C320H13CO    + hv = GLYOX + HO2 + HO2 + CO      : {%TrGJAro} jx(ip_HOCH2CHO)*2; {&2419}
<J43402> HCOCOHCO3H   + hv = GLYOX + HO2 + CO2 + OH      : {%TrGJAro} jx(ip_CH3OOH); {&2419}
<J44000a> LC4H9OOH    + hv = OH + C3H7CHO + HO2 : {%TrGJ} jx(ip_CH3OOH)*(k_p/(k_p+k_s)); {&2419, 3031}
<J44000b> LC4H9OOH    + hv = OH + .636 MEK + .636 HO2 + .364 CH3CHO + .364 C2H5O2 : {%TrGJ} jx(ip_CH3OOH)*(k_s/(k_p+k_s)); {&2419, 3031}
<J44001> MVK          + hv = .5 C3H6 + .5 CH3CO + .5 HCHO + CO + .5 HO2 : {%TrGJ} jx(ip_MVK); {&2342}
<J44002> MEK          + hv = CH3CO + C2H5O2              : {%TrGJ} 0.42*jx(ip_CHOH); {&1584}
<J44003> LMEKOOH      + hv = .62 CH3CO + .62 CH3CHO + .38 HCHO + .38 CO2 + .38 HOCH2CH2O2 + OH : {%TrGJ} jx(ip_CH3OOH)+0.42*jx(ip_CHOH); {&3031}
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<J44004>  BIACET      + hv = 2 CH3CO                      : {%TrGJ} 2.15*jx(ip_MGLYOX); // It is assumed that J(\kpp{BIACET}) is 2.15 times larger than J(\kpp{MGLYOX}), consistent with the photolysis rate coefficients used in the MCM \citep{2419}.
<J44005a> LC4H9NO3    + hv = NO2 + C3H7CHO + HO2          : {%TrGJ} J_IC3H7NO3*(k_p/(k_p+k_s)); // It is assumed that J(\kpp{LC4H9NO3}) is the same as J(\kpp{IC3H7NO3}).
<J44005b> LC4H9NO3    + hv = NO2 + MEK + HO2   : {%TrGJ} J_IC3H7NO3*(k_s/(k_p+k_s)); // It is assumed that J(\kpp{LC4H9NO3}) is the same as J(\kpp{IC3H7NO3}).
<J44006>  MPAN        + hv = .7 MACO3 + .7 NO2 + .3 MACO2 + .3 NO3                  : {%TrGJ} jx(ip_PAN); // It is assumed that J(\kpp{MPAN}) is the same as J(\kpp{PAN}).
<J44007a> CO2H3CO3H   + hv = MGLYOX + HO2 + OH   + CO2   : {%TrGJ} jx(ip_CH3OOH); {&2419}
<J44007b> CO2H3CO3H   + hv = CH3CO + HO2 + HCOCO3H : {%TrGJ} J_ACETOL; {&2419}
<J44008>  MACR        + hv = .5 MACO3 + .5 CH3CO + .5 HCHO + .5 CO + HO2   : {%TrGJ} jx(ip_MACR); {&2342}
<J44009>  MACR00H     + hv = MACRO + OH   : {%TrGJ} jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO); {&3031} // It is assumed that J(\kpp{MACR00H}) is 2.77 times larger than J(\kpp{HOCH2CHO}), consistent with the photolysis rate coefficients used in the MCM \citep{2419}.
<J44010>  MACROH      + hv = ACETOL + CO + HO2 + HO2   : {%TrGJ} 2.77*jx(ip_HOCH2CHO); // It is assumed that J(\kpp{MACROH}) is 2.77 times larger than J(\kpp{HOCH2CHO}), consistent with the photolysis rate coefficients used in the MCM \citep{2419}.
<J44011>  MACO3H      + hv = MACO2 + OH                : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44012>  LHMVKABOOH  + hv = .12 MGLYOX + .12 HO2 + .88 CH3CO + .88 HOCH2CHO + .12 HCHO + OH   : {%TrGJ} jx(ip_CH3OOH)+J_ACETOL; {&3031}
<J44013>  CO2H3CHO    + hv = MGLYOX + CO + HO2 + HO2   : {%TrGJ} jx(ip_HOCH2CHO)+J_ACETOL; {&3031}
<J44014>  HO12CO3C4   + hv = CH3CO + HOCH2CHO + HO2 : {%TrGJ} J_ACETOL; {&2419}
<J44015>  BIACETOH    + hv = CH3CO + HOCH2CO        : {%TrGJ} 2.15*jx(ip_MGLYOX); // It is assumed that J(\kpp{BIACETOH}) is 2.15 times larger than J(\kpp{MGLYOX}), consistent with the photolysis rate coefficients used in the MCM \citep{2419}.
<J44016>  HCOCCH3CO   + hv = .5 OH + .5 CH3CHO + CO + .5 CH3CHCO + .5 CO    : {%TrG} J_KETENE; {&3031}
<J44017a> CH3COCHCO   + hv = .0192 CH3COCO2H + .1848 H2O2 + .2208 MGLYOX + .36 OH + .36 CO + .56 CH3CO + .2 CH3CHO + .2 CO2 + .2 HCHO + .2 HO2 + CO   : {%TrG} J_KETENE*0.5; {&3031,2419} // CO-channel yielding \chem{CH_3COCH} which upon reaction with \kpp{O2} produces an excited Criegee Intermediate assumed to be similar to MGL00A in MCM. MGL00A is produced also in other reactions and is substituted by its decomposition products. Furthermore, the stabilized Criegge Intermediate is assumed to solely react with water.
<J44017b> CH3COCHCO   + hv = CH3CHCO + CO                                                                                                  : {%TrG} J_KETENE*0.5; {&3031}
<J44018a> CO23C3CHO   + hv = CH3CO + 2 CO + HO2           : {%TrGJ}    jx(ip_MGLYOX); {&3031}
<J44018b> CO23C3CHO   + hv = HCOCO + CH3CO                : {%TrGJ}    2.15*jx(ip_MGLYOX); {&3031}
<J44019>  CH3COCOCO2H + hv = CH3CO + CO + CO2 + HO2       : {%TrGJ}    3.15*jx(ip_MGLYOX); {&3031}
<J44020a> BIACET00H   + hv = CH3CO + OH + HCHO + CO       : {%TrGJTer} jx(ip_CH3OOH)+J_ACETOL; {&2419}
<J44020b> BIACET00H   + hv = CH3CO + HCOCO                : {%TrGJTer} 2.15*jx(ip_MGLYOX); {&2419}
<J44021>  C4400H      + hv = HCOCH2CHO + CO2 + HO2 + OH   : {%TrGJTer} jx(ip_CH3OOH); {&2419}
<J44022>  C413C000H   + hv = HCOCH2CO3 + HCHO + OH        : {%TrGJTer} jx(ip_CH3OOH)+jx(ip_HOCH2CHO)+J_ACETOL; {&2419}
<J44023a> C4CODIAL    + hv = CHOCOCH2O2 + HO2 + CO        : {%TrGJTer} jx(ip_HOCH2CHO); {&2419}
<J44023b> C4CODIAL    + hv = HCOCH2CO3 + HO2 + CO         : {%TrGJTer} jx(ip_MGLYOX); {&2419}
<J44024>  C312COCO3H  + hv = CHOCOCH2O2 + CO2 + OH        : {%TrGJTer} jx(ip_CH3OOH)+jx(ip_MGLYOX); {&2419}
<J44025>  LMEKNO3     + hv = .62 CH3CO + .62 CH3CHO + .38 HCHO + .38 CO2 + .38 HOCH2CH2O2 + NO2 : {%TrGJ} jx(ip_MEKNO3); {&3146, 3031} // J values only for the secondary nitrate.
<J44026>  MVKNO3      + hv = CH3CO + HOCH2CHO + NO2       : {%TrGJ} jx(ip_MEKNO3); {&3146, 3031} // Like for LMEKNO3 photolysis
<J44027>  MACRN       + hv = ACETOL + CO + HO2 + NO2      : {%TrGJ} (2.84*J_IC3H7NO3+jx(ip_CH3CHO))*(jx(ip_MEKNO3)+1E-10)/(J_IC3H7NO3+0.42*jx(ip_CHOH)+1E-10); {&3168, 3031} //  2.84*J\_IC3H7NO3 like for other tertiary alkyl nitrates (see J4505). Enhancement of J according to \citet{3168}.
<J44028>  TC4H9NO3    + hv = CH3COCH3 + CH3 + NO2         : {%TrGJ} 2.84*J_IC3H7NO3; {&3031}
<J44029>  TC4H9OOH    + hv = CH3COCH3 + CH3 + OH          : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44030>  IBUTOLBNO3  + hv = CH3COCH3 + HCHO + HO2 + NO2  : {%TrGJ} 2.84*J_IC3H7NO3; {&3031}
<J44031>  IBUTOLBOOH  + hv = CH3COCH3 + HCHO + HO2 + OH   : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44032>  LBUT1ENOOH  + hv = C2H5CHO + HCHO + HO2 + OH    : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44033>  LBUT1ENNO3  + hv = C2H5CHO + HCHO + HO2 + NO2   : {%TrGJ} J_IC3H7NO3; {&3031}
<J44034>  BUT2OLOOH   + hv = 2 CH3CHO + HO2 + OH          : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44035>  BUT2OLNO3   + hv = 2 CH3CHO + HO2 + NO2         : {%TrGJ} J_IC3H7NO3; {&3031}
<J44036>  BUT2OL0     + hv = CH3CO + HOCH2CO              : {%TrGJ} J_ACETOL; {&3031}
<J44037a> C3H7CHO     + hv = NC3H7O2 + CO + HO2           : {%TrGJ} jx(ip_C3H7CHO2HCO); {&3031}
<J44037b> C3H7CHO     + hv = C2H4 + CH2CHOH               : {%TrGJ} jx(ip_C3H7CHO2VINY); {&3031} // Channel which produces just vinyl alcohol and not a larger enol via keto-enol photo-tautomerization.
<J44038>  IPRCHO      + hv = IC3H7O2 + CO + HO2           : {%TrGJ} jx(ip_IPRCHO2HCO); {&3031}
<J44039>  IC4H9NO3    + hv = IPRCHO + NO2                 : {%TrGJ} J_IC3H7NO3; {&3031}
<J44040>  IC4H9OOH    + hv = IPRCHO + HO2 + OH            : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44041>  PERIBUACID  + hv = IC3H7O2 + CO2 + OH           : {%TrGJ} jx(ip_CH3OOH); {&3031}
<J44042>  PIPN        + hv = .7 IPRCO3 + .7 NO2 + .3 IC3H7O2 + .3 CO2 + .3 NO3 : {%TrGJ} jx(ip_PAN); {&3031, 2342, 2626}
<J44043>  HVMK        + hv = MGLYOX + CO + 2 OH           : {%TrGJ} jx(ip_PeDIONE24); {&3031, 3184, 3185, 3186} // The resulting vinyl peroxy radical is assumed to mostly form with \kpp{HO2} a labile hydroperoxide (see ketene formation). The products are further simplified.
<J44044>  HMAC        + hv = HCOCCH3CO + 2 OH             : {%TrGJ} jx(ip_PeDIONE24); {&3031, 3184, 3185, 3186} // 1,5-H-shift for the resulting vinyl peroxy radical assumed to be dominant.
<J44045a> CO2C3CHO    + hv = CH3COCH2O2 + HO2 + CO        : {%TrGJ} jx(ip_C2H5CHO2HCO); {&2419}
<J44045b> CO2C3CHO    + hv = HVMK                         : {%TrGJ} jx(ip_C2H5CHO2ENOL); {&3161, 3031}
<J44046a> IBUTDIAL    + hv = CH3CHO + CO + HO2 + CO2 + H2O : {%TrGJ} jx(ip_C2H5CHO2HCO)*2.; // Simplified oxidation.
<J44046b> IBUTDIAL    + hv = HMAC                         : {%TrGJ} jx(ip_C2H5CHO2ENOL)*2.; {&3161, 3031}
<J44200>  IBUTALOH    + hv = CH3COCH3 + HO2 + HO2 + CO    : {%TrGJTer} J_ACETOL; {&2419}
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<J44201>  IPRH0C03H   + hv = CH3C0CH3 + H02 + C02 + 0H     : {%TrGJTer} jx(ip_CH300H); {&2419}
<J44400a> MALDIAL00H  + hv = C3H0H13C0 + C0 + 0H + H02                  : {%TrGJAro} jx(ip_H0CH2CH0)*2; {&2419}
<J44400b> MALDIAL00H  + hv = GLY0X + GLY0X + H02 + 0H                   : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MALDIAL0 $\rightarrow$ GLY0X + GLY0X + H02
<J44401>  BZFU00H     + hv = C01403CH0 + H02 + 0H                       : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC BZFU0    $\rightarrow$ C01403CH0 + H02
<J44402>  H0C0C4DIAL  + hv = HC0C0HC03 + H02 + C0                       : {%TrGJAro} jx(ip_MGLY0X)+jx(ip_H0CH2CH0); {&2419}
<J44403>  NBZFU00H    + hv = .5 C01403CH0 + .5 N02 + .5 NBZFU0NE + .5 H02 + 0H : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NBZFU0   $\rightarrow$ .5 C01403CH0 + .5 N02 + .5 NBZFU0NE + .5 H02
<J44404a> MALDALC03H  + hv = HC0C03H + H02 + C0 + H02 + C0               : {%TrGJAro} jx(ip_MACR); {&2419}
<J44404b> MALDALC03H  + hv = .6 MALANHY + H02 + .4 GLY0X + .4 C0 + .4 C02 + 0H : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MALDIALC02 $\rightarrow$ .6 MALANHY + H02 + .4 GLY0X + .4 C0
<J44405>  EPXDLC02H   + hv = C3DIAL02 + C02 + H02                       : {%TrGJAro} 2.77*jx(ip_H0CH2CH0); {&2419}
<J44406>  MALDIAL     + hv = .4 BZFU0NE + .6 MALDIALC03 + .6 H02        : {%TrGJAro} jx(ip_N02)*0.14; {&2419}
<J44407>  MALANHY00H  + hv = HC0C0HC03 + C02 + 0H                       : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MALANHY0 $\rightarrow$ HC0C0HC03
<J44408>  EPXDLC03H   + hv = C3DIAL02 + 0H + C02                        : {%TrGJAro} jx(ip_CH300H)+2.77*jx(ip_H0CH2CH0); {&2419}
<J44409>  C02C4DIAL   + hv = C0 + C0 + H02 + H02 + C0 + C0              : {%TrGJAro} jx(ip_MGLY0X)*2; {&2419}
<J44410>  MALDALC02H  + hv = HC0C02H + H02 + C0 + H02 + C0              : {%TrGJAro} jx(ip_MACR); {&2419}
<J44411>  EPXC4DIAL   + hv = C3DIAL02 + C0 + H02                        : {%TrGJAro} 2.77*jx(ip_H0CH2CH0)*2; {&2419}
<J44412>  C01403CH0   + hv = H02 + C0 + HC0CH202 + C02                  : {%TrGJAro} jx(ip_MGLY0X); {&2419}
<J44414>  MEC0ACE00H  + hv = CH3C0 + HCH0 + C02 + 0H                    : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MEC0ACET0 $\rightarrow$ CH3C03 + HCH0
<J45002>  LIS0PAC00H  + hv = LIS0PAC0 + 0H      : {%TrGJ} jx(ip_CH300H); {&2419}
<J45003>  LIS0PACN03  + hv = LIS0PAC0 + N02   : {%TrGJ} 0.59*J_IC3H7N03; // It is assumed that J(\kpp{LIS0PACN03}) = 0.59 $\times$ J(\kpp{IC3H7N03}), consistent with the photolysis rate coefficients used in the MCM \citep{2419}.
<J45004>  IS0PB00H    + hv = MVK + HCH0 + H02 + 0H     : {%TrGJ} jx(ip_CH300H); {&2419}
<J45005>  IS0PBN03    + hv = MVK + HCH0 + H02 + N02  : {%TrGJ} 2.84*J_IC3H7N03; // It is assumed that J(\kpp{IS0PBN03}) = 2.84 $\times$ J(\kpp{IC3H7N03}), consistent with the photolysis rate coefficients used in the MCM \citep{2419}.
<J45006>  IS0PD00H    + hv = MACR + HCH0 + H02 + 0H                                 : {%TrGJ} jx(ip_CH300H); {&2419}
<J45007>  IS0PDN03    + hv = MACR + HCH0 + H02 + N02                                : {%TrGJ} J_IC3H7N03; // It is assumed that J(\kpp{IS0PDN03}) is the same as J(\kpp{IC3H7N03}).
<J45008>  NIS0P00H    + hv = NC4CH0 + H02 + 0H                                      : {%TrGJ} jx(ip_CH300H); {&2419}
<J45009>  NC4CH0      + hv = LHC4ACC03 + N02                                        : {%TrGJ} (.59*J_IC3H7N03+jx(ip_MACR))*(jx(ip_MEKN03)+1E-10)/(J_IC3H7N03+0.42*jx(ip_CH0H)+1E-10); {&3168, 3031} //  0.59*J\_IC3H7N03 like for other primary alkyl nitrates (see J4503). Enhancement of J according to \citet{3168}.
<J45010>  LNIS00H     + hv = N0A + 0H + .5 H0CHCH0 + .5 C0 + .5 H02 + .5 C02        : {%TrGJ} jx(ip_CH300H); {&2272, 3031}
<J45011>  LHC4ACCH0   + hv = .5 LHC4ACC03 + .5 H02 + .5 C0 + .5 0H + .25 MACR02 + .25 LHMVKAB02    : {%TrGJ} jx(ip_MACR); {&3031}
<J45012>  LC57800H    + hv = .25 ACETOL + .75 MGLY0X + .25 H0CHCH0 + .75 H0CH2CH0 + .75 H02 + 0H   : {%TrGJ} jx(ip_CH300H)+ 2.77*jx(ip_H0CH2CH0); {&3031}
<J45013>  LHC4ACC03H  + hv = 0H + .5 MACR02 + .5 LHMVKAB02 + 0H  + C02              : {%TrGJ} J_HPALD; {&3031}
<J45014>  LC5PAN1719  + hv = .7 LHC4ACC03  + .7 N02 + .15 MACR02 + .15 LHMVKAB02 + .3 C02 + .3 N03 : {%TrGJ} jx(ip_PAN); {&3031}
<J45015>  HC0C5       + hv = .65 CH3 + .65 C0 + .65 HCH0 + .35 0H + .35 CH3C0CH202 + H0CH2C0 : {%TrGJ} 0.5*jx(ip_MVK); {&3031} // Consistent with the MCM \citep{2419}, we assume that J(\kpp{HC0C5}) is half as large as J(\kpp{MVK}). With exception of \kpp{H0CH2C0} the products of \kpp{MAC02} decomposition without \kpp{C02}.
<J45016>  C5900H      + hv = ACETOL + H0CH2C0 + 0H             : {%TrGJ}    J_ACETOL+jx(ip_CH300H); {&3031}
<J45017>  C51100H     + hv = CH3C0 + HC0CH2CH0 + 0H            : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J45018a> C023C4CH0   + hv = BIACET02 + H02 + C0               : {%TrGJTer} jx(ip_H0CH2CH0); {&2419}
<J45018b> C023C4CH0   + hv = CH3C0 + HC0CH2C03                 : {%TrGJTer} 2.15*jx(ip_MGLY0X); {&2419}
<J45019>  C023C4C03H  + hv = BIACET02 + C02 + 0H               : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J45020>  C51200H     + hv = C51302 + 0H                       : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J45021>  C013C4CH0   + hv = CH0C3C002 + C0 + H02              : {%TrGJTer} jx(ip_H0CH2CH0)*2.; {&2419}
<J45022>  C51300H     + hv = GLY0X + H0C2H4C03 + 0H            : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J45023>  C513C0      + hv = H0C2H4C03 + H02 + C0 + C0         : {%TrGJTer} jx(ip_MGLY0X)+2.15*jx(ip_MGLY0X); {&2419}
<J45024>  C51400H     + hv = C013C4CH0 + H02 + 0H              : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0)*2.; {&2419}
<J45025>  C514N03     + hv = C013C4CH0 + H02 + N02             : {%TrGJTer} J_IC3H7N03+jx(ip_H0CH2CH0)*2.; {&2419}
<J45026a> ZC0DC23DBC00H  + hv = 0H + C0 + HVMK + 0H            : {%TrGJ} J_HPALD*0.6*0.5; {&3031, 3182, 3183}
<J45026b> ZC0DC23DBC00H  + hv = 0H + C0 + CH3C0 + H0CH2CH0     : {%TrGJ} J_HPALD*0.6*0.5; {&3031, 3182, 3183}
<J45026c> ZC0DC23DBC00H  + hv = 0H + C0 + HMAC + 0H            : {%TrGJ} J_HPALD*0.4*0.5; {&3031, 3182, 3183}
<J45026d> ZC0DC23DBC00H  + hv = 0H + C0 + C0 + ACETOL + H02    : {%TrGJ} J_HPALD*0.4*0.5; {&3031, 3182, 3183}
<J45027>  ZC03HC23DBC0D  + hv = .62 EZCH3C02CHCH0 + .38 EZCH0CCH3CH02 + 0H + C02              : {%TrGJ} J_HPALD; {&3031}
<J45028a> C100HC200HC40D + hv = HYPERACET + 0H + 2 C0 + H02                                   : {%TrGJ} 2.77*JX(IP_H0CH2CH0); {&3031}
<J45028b> C100HC200HC40D + hv = .5 HYPERACET + .5 H0CHCH0 + .5 C02H3CH0 + .5 HCH0 + 1.5 0H   : {%TrGJ} 2.*JX(IP_CH300H); {&3031}
<J45029>  DB100H         + hv = DB10 + 0H                                                     : {%TrG} JX(IP_CH300H); {&3031}
<J45030>  DB200H         + hv = .48 ACETOL + .52 H0CH2CH0 + .52 MGLY0X + .48 GLY0X + H02 + 0H  : {%TrG} JX(ip_CH300H); {&3031}
<J45031a> C10DC200HC40D  + hv = MGLY0X + H0CHCH0 + 0H                                         : {%TrGJ} JX(ip_CH300H); {&3031}
<J45031b> C10DC200HC40D  + hv = C02H3CH0 + C0 + H02 + 0H                                      : {%TrGJ} 2.*2.77*JX(IP_H0CH2CH0); {&3031}
<J45032>  ZC0DC23DBC0D   + hv = .5 CH3C0CHC0 + .5 HC0CCH3C0 + C0 + H02 + 0H                  : {%TrGJ} jx(ip_N02)*0.1*0.5; {&3031} //{approximation with 4-oxo-pentenal photolysis combining results of ThÃ¼ner et al(2004) and Xiang et al(2007)}
<J45033>  DB1N03      + hv = DB10 + N02                        : {%TrG} J_IC3H7N03; {&3031}
<J45034>  CH0C3C000H  + hv = CH0C3C002 +C02 + 0H               : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0)+J_ACETOL; {&2419}
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<J45200a> LMB0AB00H   + hv = H0CH2CH0 + CH3C0CH3 + H02 + 0H    : {%TrGJTer} jx(ip_CH300H)*.67; {&2419, 3031}
<J45200b> LMB0AB00H   + hv = IBUTAL0H + HCH0 + H02 + 0H        : {%TrGJTer} jx(ip_CH300H)*.33; {&2419, 3031}
<J45201>  MB0AC0      + hv = HCH0 + H02 + IPRH0C03             : {%TrGJTer} J_ACET0L; {&2419}
<J45202>  MB0C0C0     + hv = C0 + H02 + IPRH0C03               : {%TrGJTer} jx(ip_MGLY0X); {&2419}
<J45203a> LNMB0AB00H  + hv = N03CH2CH0 + CH3C0CH3 + H02 + 0H   : {%TrGJTer} jx(ip_CH300H)*.65; {&2419, 3031}
<J45203b> LNMB0AB00H  + hv = IBUTAL0H + HCH0 + N02 + 0H        : {%TrGJTer} jx(ip_CH300H)*.35; {&2419, 3031}
<J45204>  NC40HC03H   + hv = IBUTAL0H + C02 + N02 + 0H         : {%TrGJTer} jx(ip_CH300H); {&2419}
<J45400>  C54C0       + hv = H02 + C0 + C0 + C0 + CH3C0        : {%TrGJAro} jx(ip_MGLY0X)+2.15*jx(ip_MGLY0X)*2; {&2419}
<J45401>  C5134C020H  + hv = C023C3CH0 + H02 + C0 + H02        : {%TrGJAro} jx(ip_H0CH2CH0)+2.15*jx(ip_MGLY0X); {&2419}
<J45402>  C5DIAL00H   + hv = MALDIAL + C0 + H02 + 0H           : {%TrGJAro} jx(ip_CH300H)+jx(ip_MACR); {&2419} // KDEC C5DIAL0 $\rightarrow$ MALDIAL + C0 + H02
<J45406>  C5C0140H    + hv = CH3C0 + HC0C02H + H02 + C0        : {%TrGJAro} jx(ip_MVK); {&2419}
<J45407>  C5DICARB    + hv = .6 C5C01402 + .6 H02 + .4 TLFU0NE : {%TrGJAro} jx(ip_N02)*0.2; {&2419} // KDEC TLFU0NE $\rightarrow$ .6 C5C01402 + .6 H02 + .4 TLFU0NE
<J45408>  MC30DBC02H  + hv = CH3C0C02H + H02 + C0 + H02 + C0   : {%TrGJAro} jx(ip_MACR); {&2419}
<J45409>  ACC0MECH0   + hv = MEC0ACET02 + H02 + C0             : {%TrGJAro} jx(ip_H0CH2CH0); {&2419}
<J45410>  MMALNHY00H  + hv = C02H3C03 + C02 + 0H               : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MMALANHY0 $\rightarrow$ C02H3C03
<J45411>  C5DICAR00H  + hv = MGLY0X + GLY0X + H02 + 0H         : {%TrGJAro} jx(ip_CH300H)+jx(ip_H0CH2CH0)+J_ACET0L; {&2419} // KDEC C5DICARB0 $\rightarrow$ MGLY0X + GLY0X + H02
<J45412>  NTLFU00H    + hv = ACC0MECH0 + N02 + 0H              : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NTLFU0    $\rightarrow$ ACC0MECH0 + N02
<J45414>  C5C01400H   + hv = .83 MALANHY + .83 CH3 + .17 MGLY0X + .17 H02 + .17 C0 + .17 C02 + 0H : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC C5C014C02  $\rightarrow$ .83 MALANHY + .83 CH3 + .17 MGLY0X +
.17 H02 + .17 C0 + .17 C02
<J45415>  TLFU00H     + hv = ACC0MECH0 + H02 + 0H              : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC TLFU0 $\rightarrow$ ACC0MECH0 + H02
<J45417>  ACC0MEC03H  + hv = MEC0ACET02 + C02 + 0H             : {%TrGJAro} jx(ip_CH300H); {&2419}
<J45418>  C5DIALC0    + hv = MALDIALC03 + C0 + H02             : {%TrGJAro} jx(ip_MGLY0X)+jx(ip_MACR); {&2419}
<J46200>  C614N03     + hv = C023C4CH0 + HCH0 + H02 + N02      : {%TrGJTer} 2.15*jx(ip_MGLY0X); {&2419}
<J46201>  C61400H     + hv = C023C4CH0 + HCH0 + H02 + 0H       : {%TrGJTer} jx(ip_CH300H)+2.15*jx(ip_MGLY0X); {&2419}
<J46202>  C0235C5CH0  + hv = C023C4C03 + C0 + H02              : {%TrGJTer} jx(ip_MGLY0X); {&2419}
<J46203>  C0235C600H  + hv = C023C4C03 + HCH0 + 0H             : {%TrGJTer} jx(ip_CH300H)+2.15*jx(ip_MGLY0X); {&2419}
<J46400>  PHEN00H     + hv = .71 MALDALC02H + .71 GLY0X + .29 PBZ@0NE + H02 + 0H : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC PHEN0 $\rightarrow$ .71 MALDALC02H + .71 GLY0X + .29 PBZ@0NE + H02
<J46401>  C6C04DB     + hv = C4C02DBC03 + H02 + C0             : {%TrGJAro} jx(ip_MGLY0X)*2; {&2419}
<J46402>  C5C02DC03H  + hv = CH3C0 + C33C0 + C02 + 0H          : {%TrGJAro} jx(ip_CH300H)+jx(ip_MGLY0X); {&2419}
<J46403>  NDNPHEN00H  + hv = NC4DC02H + HN03 + C0 + C0 + N02 + 0H       : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NDNPHEN0 $\rightarrow$ NC4DC02H + HN03 + C0 + C0 + N02
<J46404>  BZBIPERN03  + hv = GLY0X + H02 + .5 BZFU0NE + .5 BZFU0NE + N02 : {%TrGJAro} J_IC3H7N03; {&2419} // KDEC BZBIPER0 $\rightarrow$ GLY0X + H02 + .5 BZFU0NE + .5 BZFU0NE
<J46405>  H0C6H4N02   + hv = H0N0 + CPDKETENE                  : {%TrGJAro} jx(ip_H0C6H4N02); {&3203} //new channel created for nitrophenol decomposition
<J46406>  CPDKETENE   + hv = C02 + C0 + 2 H02 + MALDIAL        : {%TrGJAro} J_KETENE; //new channel created for nitrophenol decomposition
<J46407>  C5C00HC03H  + hv = H0C0C4DIAL + H02 + C0 + C02 + 0H  : {%TrGJAro} jx(ip_CH300H); {&2419}
<J46408>  BZEP0XMUC   + hv = .5 C5DIAL02 + 1.5 H02 + 1.5 C0 + .5 MALDIAL : {%TrGJAro} 4.E3*jx(ip_MVK)*0.1; {&2419}
<J46409>  NPHEN100H   + hv = NPHEN10 + 0H                      : {%TrGJAro} jx(ip_CH300H); {&2419}
<J46410>  BZEMUCC0    + hv = HC0C0HC03 + C3DIAL02              : {%TrGJAro} jx(ip_H0CH2CH0)*2+J_ACET0L; {&2419}
<J46411>  BZEMUCC02H  + hv = C5DIAL02 + C02 + H02              : {%TrGJAro} jx(ip_MACR); {&2419}
<J46412>  NNCATEC00H  + hv = NC4DC02H + HC0C02H + N02 + 0H     : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NNCATEC0 $\rightarrow$ NC4DC02H + HC0C02H + N02
<J46413>  C615C0200H  + hv = C5DICARB + C0 + H02 + 0H          : {%TrGJAro} jx(ip_MVK)+jx(ip_CH300H); {&2419}
<J46414>  NPHEN00H    + hv = MALDALC02H + GLY0X + 0H + N02     : {%TrGJAro} J_IC3H7N03 + jx(ip_CH300H); {&2419}
<J46415>  NCATEC00H   + hv = NC4DC02H + HC0C02H + H02 + 0H     : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NCATEC0 $\rightarrow$ NC4DC02H + HC0C02H + H02
<J46416>  PBZ@00H     + hv = C5C020HC03 + 0H                   : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC PBZ@0 $\rightarrow$ C5C020HC03
<J46417>  BZ0BIPER0H  + hv = MALDIALC03 + GLY0X + H02          : {%TrGJAro} J_ACET0L; {&2419}
<J46418>  BZBIPER00H  + hv = GLY0X + H02 + .5 BZFU0NE + .5 BZFU0NE + 0H : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC BZBIPER0 $\rightarrow$ GLY0X + H02 + .5 BZFU0NE + .5 BZFU0NE
<J46419>  NBZ@00H     + hv = C6C04DB + N02 + 0H                : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NBZ@0 $\rightarrow$ C6C04DB + N02
<J46420>  CATEC100H   + hv = CATEC10 + 0H                      : {%TrGJAro} jx(ip_CH300H); {&2419}
<J46421>  C61254C0    + hv = C5C01402 + C0 + H02               : {%TrGJAro} jx(ip_MGLY0X)+jx(ip_MVK); {&2419}
<J46422>  DNPHEN00H   + hv = NC4DC02H + HC0C02H + N02 + 0H     : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC DNPHEN0 $\rightarrow$ NC4DC02H + HC0C02H + N02
<J46423>  BZEMUCC03H  + hv = C5DIAL02 + C02 + 0H               : {%TrGJAro} jx(ip_CH300H)+jx(ip_MACR); {&2419}
<J46424>  C6H500H     + hv = C6H50 + 0H                        : {%TrGJAro} jx(ip_CH300H); {&2419}
<J46425>  BZEMUC00H   + hv = .5 EPXC4DIAL + .5 GLY0X + .5 H02 + .5 C3DIAL02 + .5 C320H13C0 + 0H : {%TrGJAro} jx(ip_CH300H)+jx(ip_H0CH2CH0)*2; {&2419} // KDEC BZEMUC0 $\rightarrow$ .5 EPXC4DIAL + .5 GLY0X +
.5 H02 + .5 C3DIAL02 + .5 C320H13C0
<J46427>  BZEMUCN03   + hv = EPXC4DIAL + N02 + GLY0X + H02     : {%TrGJAro} 2.77*jx(ip_H0CH2CH0); {&2419}
<J46428>  DNPHEN      + hv = H0N0 + NCPDKETENE                 : {%TrGJAro} jx(ip_H0C6H4N02); {&3031}
<J46429>  NCPDKETENE  + hv = C02 + C0 + 2 H02 + NC4DC02H       : {%TrGJAro} J_KETENE; //new channel
<J47200>  C0235C6CH0  + hv = CH0C3C0C03 + CH3C0          : {%TrGJTer} 2.15*jx(ip_MGLY0X); {&2419}
<J47201>  C235C6C03H  + hv = C0235C602 + C02 + 0H         : {%TrGJTer} jx(ip_CH300H)+2.15*jx(ip_MGLY0X); {&2419}
<J47202>  C71600H     + hv = C013C4CH0 + CH3C0 + 0H       : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J47203>  C72100H     + hv = C72202 + 0H                  : {%TrGJTer} jx(ip_CH300H); {&2419}
<J47204>  C72200H     + hv = CH3C0CH3 + C4402 + 0H        : {%TrGJTer} jx(ip_CH300H); {&2419}
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<J47400>  TLEP0XMUC   + hv = .5 C615C0202 + H02 + C0 + .5 EPXC4DIAL + .5 CH3C0 : {%TrGJAro} 4.E3*jx(ip_MVK)*0.1; {&2419}
<J47401>  C6H5CH200H  + hv = BENZAL + H02 + 0H                        : {%TrGJAro} jx(ip_CH300H); {&2419} // KR0PRIM*02 fast reaction C6H5CH20 = BENZAL + H02
<J47402>  C6H5CH2N03  + hv = BENZAL + H02 + N02                       : {%TrGJAro} 0.59*J_IC3H7N03; {&2419} // KR0PRIM*02 fast reaction C6H5CH20 = BENZAL + H02
<J47403>  BENZAL      + hv = H02 + C0 + C6H502                        : {%TrGJAro} jx(ip_BENZAL); {&1745}
<J47404>  TLBIPER00H  + hv = .6 GLY0X + .4 MGLY0X + H02 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFU0NE + .2 BZFU0NE + .2 MALDIAL + 0H : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC TLBIPER0 $\rightarrow$ .6
GLY0X + .4 MGLY0X + H02 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFU0NE + .2 BZFU0NE + .2 MALDIAL
<J47405>  TLBIPERN03  + hv = .6 GLY0X + .4 MGLY0X + H02 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFU0NE + .2 BZFU0NE + .2 MALDIAL + N02 : {%TrGJAro} J_IC3H7N03; {&2419} // KDEC TLBIPER0 $\rightarrow$ .6 GLY0X
+ .4 MGLY0X + H02 + .2 ZC0DC23DBC0D + .2 C5DICARB + .2 TLFU0NE + .2 BZFU0NE + .2 MALDIAL
<J47406>  TL0BIPER0H  + hv = C5C01402 + GLY0X + H02                   : {%TrGJAro} J_ACET0L; {&2419}
<J47407>  CRES00H     + hv = .68 C5C0140H + .68 GLY0X + H02 + .32 PTL0NE + 0H  : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC CRES0 $\rightarrow$ .68 C5C0140H + .68 GLY0X + H02 + .32 PTL0NE
<J47408a> NCRES00H    + hv = .68 C5C0140H + .68 GLY0X + H02 + .32 PTL0NE + 0H + N02 : {%TrGJAro} J_IC3H7N03; {&2419} // KDEC CRES0 $\rightarrow$ .68 C5C0140H + .68 GLY0X + H02 + .32 PTL0NE
<J47408b> NCRES00H    + hv = C5C0140H + GLY0X + N02  + 0H             : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NCRES0 $\rightarrow$ C5C0140H + GLY0X + N02
<J47409>  T0L10HN02   + hv = H0N0 + MCPDKETENE                        : {%TrGJAro} jx(ip_H0Ph3Me2N02); // Using J for 3-methyl-2-nitrophenol.
<J47410>  TLEMUCC02H  + hv = C615C0202 + C02 + H02                    : {%TrGJAro} jx(ip_MACR); {&2419}
<J47411>  TLEMUCC03H  + hv = C615C0202 + C02 + 0H                     : {%TrGJAro} jx(ip_CH300H)+jx(ip_MACR); {&2419}
<J47412>  TLEMUC00H   + hv = .5 C3DIAL02 + .5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02 + 0H : {%TrGJAro} jx(ip_CH300H)+2.77*jx(ip_H0CH2CH0)+J_ACET0L; {&2419} // KDEC TLEMUC0 $\rightarrow$ .5 C3DIAL02 +
.5 C02H3CH0 + .5 EPXC4DIAL + .5 MGLY0X + .5 H02
<J47413>  TLEMUCN03   + hv = EPXC4DIAL + N02 + CH3C0 + C0 + H02       : {%TrGJAro} 2.77*jx(ip_H0CH2CH0)+J_ACET0L; {&2419}
<J47414>  TLEMUCC0    + hv = CH3C0 + EPXC4DIAL + C0 + H02             : {%TrGJAro} 2.77*jx(ip_H0CH2CH0)+2.15*jx(ip_MGLY0X); {&2419}
<J47415>  C6H5C03H    + hv = C6H502 + C02 + 0H                        : {%TrGJAro} jx(ip_CH300H); {&2419}
<J47416>  0XYL10OH    + hv = T0L10 + 0H                               : {%TrGJAro} jx(ip_CH300H); {&2419}
<J47417>  MNCATECH    + hv = H0N0 + MCPDKETENE                        : {%TrGJAro} jx(ip_H0Ph3Me2N02); // Using J for 3-methyl-2-nitrophenol.
<J47418>  MCPDKETENE  + hv = C02 + C0 + 2 H02 + ZC0DC23DBC0D          : {%TrGJAro} J_KETENE; //new channel
<J47419>  DNCRES      + hv = H0N0 + MNCPDKETENE                       : {%TrGJAro} jx(ip_H0Ph3Me2N02); // Using J for 3-methyl-2-nitrophenol.
<J47420>  MNCPDKETENE + hv = C02 + C0 + 2 H02 + NC4MDC02H            : {%TrGJAro} J_KETENE; //new channel
<J47421>  MCATEC10OH  + hv = MCATEC10 + 0H                            : {%TrGJAro} jx(ip_CH300H); {&2419}
<J47422>  NPTL00OH    + hv = C7C04DB + N02 + 0H                       : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NPTL00 $\rightarrow$ C7C04DB + N02
<J47423>  PTL00OH     + hv = C6C020HC03 + 0H                          : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC PTL00 $\rightarrow$ C6C020HC03
<J47424>  NCRES100H   + hv = NCRES10 + 0H                             : {%TrGJAro} jx(ip_CH300H); {&2419}
<J47425>  MNNCATC00H  + hv = NC4MDC02H + HC0C02H + N02 + 0H           : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MNNCATEC0 $\rightarrow$ NC4MDC02H + HC0C02H + N02
<J47426>  MNCATEC00H  + hv = NC4MDC02H + HC0C02H + H02 + 0H           : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC MNCATEC0 $\rightarrow$ NC4MDC02H + HC0C02H + H02
<J47427>  C7C04DB     + hv = C5C02DBC03 + H02 + C0                    : {%TrGJAro} jx(ip_MGLY0X)*2; {&2419}
<J47428>  NDNCRES00H  + hv = NC4MDC02H + HN03 + C0 + C0 + N02 + 0H    : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC NDNCRES0 $\rightarrow$ NC4MDC02H + HN03 + C0 + C0 + N02
<J47429>  DNCRES00H   + hv = NC4MDC02H + HC0C02H + N02 + 0H           : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC DNCRES0 $\rightarrow$ NC4MDC02H + HC0C02H + N02
<J47430>  C6C00HC03H  + hv = C5134C020H + H02 + C0 + C02 + 0H         : {%TrGJAro} jx(ip_CH300H); {&2419}
<J48200>  C8600H      + hv = C5110Z + CH3C0CH3 + 0H        : {%TrGJTer} jx(ip_CH300H)+ jx(ip_H0CH2CH0); {&2419}
<J48201>  C81200H     + hv = C8130Z + 0H                   : {%TrGJTer} jx(ip_CH300H); {&2419}
<J48202>  C81300H     + hv = CH3C0CH3 + C5120Z + 0H        : {%TrGJTer} jx(ip_CH300H)+jx(ip_MGLY0X); {&2419}
<J48203>  C721CH0     + hv = C7210Z + C0 + H02             : {%TrGJTer} jx(ip_H0CH2CH0); {&2419}
<J48204>  C721C03H    + hv = C7210Z + C02 + 0H             : {%TrGJTer} jx(ip_CH300H); {&2419}
<J48205>  C8BC00H     + hv = C8902 + 0H                    : {%TrGJTer} jx(ip_CH300H); {&2419}
<J48206>  C8900H      + hv = C8100Z + 0H                   : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J48207>  C89N03      + hv = C8100Z + N02                  : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J48208>  C810O0H     + hv = CH3C0CH3 + C5140Z + 0H        : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J48209>  C810N03     + hv = CH3C0CH3 + C5140Z + N02       : {%TrGJTer} 2.84*J_IC3H7N03+jx(ip_H0CH2CH0); {&2419}
<J48210>  C8BCN03     + hv = C8902 + N02                   : {%TrGJTer} J_IC3H7N03; {&2419}
<J48211>  C8500H      + hv = C8602 + 0H                    : {%TrGJTer} jx(ip_CH300H)+J_ACET0L; {&2419}
<J48400>  STYREN00H   + hv = H02 + HCH0 + BENZAL + 0H      : {%TrGJAro} jx(ip_CH300H); {&2419} // KDEC STYREN0 $\rightarrow$ H02 + HCH0 + BENZAL
<J49200>  C9600H      + hv = C9702 + 0H                    : {%TrGJTer} jx(ip_CH300H)+J_ACET0L; {&2419}
<J49201>  C9700H      + hv = C9802 + 0H                    : {%TrGJTer} jx(ip_CH300H)+J_ACET0L; {&2419}
<J49202>  C9800H      + hv = C6140Z + CH3C0CH3 + 0H        : {%TrGJTer} (jx(ip_CH300H)+2.15*jx(ip_MGLY0X)); {&2419}
<J49203a> N0RPINAL    + hv = C8502 + C0 + H02              : {%TrGJTer} jx(ip_PINAL2HC0); {&2419, 3031}
<J49203b> N0RPINAL    + hv = N0RPINEN0L                    : {%TrGJTer} jx(ip_PINAL2EN0L); {&3031, 3161}
<J49204>  C85C03H     + hv = C8502 + C02 + 0H              : {%TrGJTer} jx(ip_CH300H)+J_ACET0L; {&2419}
<J49205>  C89C02H     + hv = .8 C811C03 + .2 C8902 + .2 C02 + H02 : {%TrGJTer} jx(ip_H0CH2CH0); {&2419}
<J49206>  C89C03H     + hv = .8 C811C03 + .2 C8902 + .2 C02 + 0H  : {%TrGJTer} jx(ip_CH300H)+jx(ip_H0CH2CH0); {&2419}
<J49207>  C811C03H    + hv = C8110Z + C02 + 0H             : {%TrGJTer} jx(ip_CH300H); {&2419}
<J49208>  N0PIND00H   + hv = C89C03 + 0H                   : {%TrGJTer} jx(ip_CH300H); {&2419}
<J40200>  LAPINAB00H     + hv = PINAL + H02 + 0H             : {%TrGJTer} jx(ip_CH300H); {&2419}
<J40201>  MENTHEN6ONE    + hv = R06R102 + 0H                 : {%TrGJTer} jx(ip_CH300H); {&3017}
<J40202>  0H2MENTHEN6ONE + hv = 10 LCARB0N + 0H              : {%TrGJTer} jx(ip_CH300H); {&3017}
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<J40203a> PINAL          + hv = CH3O2 + CO + HO2            : {%TrGJTer} jx(ip_PINAL2HCO); {&2419}
<J40203b> PINAL          + hv = PINENOL                     : {%TrGJTer} jx(ip_PINAL2ENOL); {&3031, 3161} // Substituted vinyl alcohol in analogy to \kpp{CH3CHO} photolysis.
<J40204>  PERPINONIC     + hv = CH3O2 + CO2 + OH            : {%TrGJTer} jx(ip_CH3OOH)+J_ACETOL; {&2419}
<J40205>  PINALOOH       + hv = C10O2 + OH                  : {%TrGJTer} jx(ip_CH3OOH)+jx(ip_HOCH2CHO); {&2419}
<J40206>  PINALNO3       + hv = C10O2 + NO2                 : {%TrGJTer} J_IC3H7NO3+jx(ip_HOCH2CHO); {&2419}
<J40207>  C10O6OH        + hv = C7H6O2 + CH3COCH3 + OH      : {%TrGJTer} jx(ip_CH3OOH)+jx(ip_HOCH2CHO); {&2419}
<J40208>  C10O6NO3       + hv = C7H6O2 + CH3COCH3 + NO2     : {%TrGJTer} J_IC3H7NO3+ jx(ip_HOCH2CHO); {&2419}
<J40209>  C10OOOH        + hv = C8H8O3 + HCHO + OH          : {%TrGJTer} jx(ip_CH3OOH)+jx(ip_HOCH2CHO); {&2419}
<J40210>  C10H8O         + hv = C8H8O3 + CO + HO2           : {%TrGJTer} jx(ip_MGLYOX)+jx(ip_HOCH2CHO); {&2419}
<J40211>  LNAPINABOOH    + hv = PINAL + NO2 + OH            : {%TrGJTer} jx(ip_CH3OOH); {&2419}
<J40212>  BPINAOOH       + hv = NOPINONE + HCHO + HO2 + OH  : {%TrGJTer} jx(ip_CH3OOH); {&2419}
<J40213>  LNBPINABOOH    + hv = NOPINONE + HCHO + NO2 + OH  : {%TrGJTer} jx(ip_CH3OOH); {&2419}
<J40214>  RO0ONO3        + hv = RO0O2R302 + CH3CO2CH3 + NO2 : {%TrGJTer} 2.84*J_IC3H7NO3+jx(ip_CH3OOH); {&3031}
<J40215>  RO6R1NO3       + hv = 9 LCARBON + HCHO + HO2 + NO2 : {%TrGJTer} 2.84*J_IC3H7NO3; {&3031}
{<J5nnn> ------------------------------ F ------------------------}{@\myhline}
{<J6nnn> ------------------------------ Cl -----------------------}{@\myhline}
<J60001>  Cl2     + hv = Cl + Cl              : {%StTrGJ}  jx(ip_Cl2); {&2342}
<J61001>  Cl2O2   + hv = 2 Cl                 : {%StTrGJ}  jx(ip_Cl2O2); {&2342}
<J61101>  OClO    + hv = ClO + O3P            : {%StTrGJ}  jx(ip_OClO); {&2342}
<J62001>  HCl     + hv = Cl + H               : {%StGJ}    jx(ip_HCl); {&2342}
<J62101>  HOCl    + hv = OH + Cl              : {%StTrGJ}  jx(ip_HOCl); {&2342}
<J63001>  ClNO2   + hv = Cl + NO2             : {%TrGJ}    jx(ip_ClNO2); {&2342}
<J6301a>  ClNO3   + hv = Cl + NO3             : {%StTrGJ}  jx(ip_ClNO3); {&2342}
<J6301b>  ClNO3   + hv = ClO + NO2            : {%StTrGJ}  jx(ip_ClONO2); {&2342}
<J64001>  CH3Cl   + hv = Cl + CH3             : {%StGJ}    jx(ip_CH3Cl); {&2342}
<J64101>  CCl4    + hv = LCARBON + 4 Cl       : {%StGJ}    jx(ip_CCl4); {&2342}
<J64102>  CH3CCl3 + hv = 2 LCARBON + 3 Cl     : {%StGJ}    jx(ip_CH3CCl3); {&2342}
<J65001>  CFCl3   + hv = LCARBON + LFLUORINE + 3 Cl   : {%StGJ} jx(ip_CFCl3); {&2342}
<J65101>  CF2Cl2  + hv = LCARBON + 2 LFLUORINE + 2 Cl : {%StGJ} jx(ip_CF2Cl2); {&2342}
{<J7nnn> ------------------------------ Br -----------------------}{@\myhline}
<J70001>  Br2     + hv = Br + Br              : {%StTrGJ}  jx(ip_Br2); {&2342}
<J71001>  BrO     + hv = Br + O3P             : {%StTrGJ}  jx(ip_BrO); {&2342}
<J72001>  HOBr    + hv = Br + OH              : {%StTrGJ}  jx(ip_HOBr); {&2342}
<J73001>  BrNO2   + hv = Br + NO2             : {%TrGJ}    jx(ip_BrNO2); {&2342}
<J73101>  BrNO3   + hv = .85 Br + .85 NO3 + .15 BrO + .15 NO2 : {%StTrGJ} jx(ip_BrNO3); {&2342} // The quantum yields are recommended by \citet{2626} for $\lambda > 300 \unit{nm}$ and used here for the
entire spectrum.
<J74001>  CH3Br   + hv = Br + CH3                : {%StGJ} jx(ip_CH3Br); {&2342}
<J74101>  CH2Br2  + hv = LCARBON + 2 Br {+CH3O2} : {%TrGJ} jx(ip_CH2Br2); {&2342}
<J74102>  CHBr3   + hv = LCARBON + 3 Br {+CH3O2} : {%TrGJ} jx(ip_CHBr3); {&2342}
<J75001>  CF3Br   + hv = LCARBON + 3 LFLUORINE + Br   : {%StGJ} jx(ip_CF3Br); {&2342}
<J76001>  BrCl    + hv = Br + Cl                      : {%StTrGJ} jx(ip_BrCl); {&2342}
<J76101>  CF2ClBr + hv = LCARBON + 2 LFLUORINE + Br + Cl : {%StGJ}   jx(ip_CF2ClBr); {&2342}
<J76102>  CH2ClBr + hv = LCARBON + Br + Cl   {+CH3O2}    : {%TrGJ}   jx(ip_CH2ClBr); {&2342}
<J76103>  CHCl2Br + hv = LCARBON + Br + 2 Cl {+CH3O2}    : {%TrGJ}   jx(ip_CHCl2Br); {&2342}
<J76104>  CHClBr2 + hv = LCARBON + 2 Br + Cl {+CH3O2}    : {%TrGJ}   jx(ip_CHClBr2); {&2342}
{<J8nnn> ------------------------------ I ------------------------}{@\myhline}
<J80001>  I2      + hv = I + I                : {%TrGJ}  jx(ip_I2); {&2342}
<J81001>  IO      + hv = I + O3P              : {%TrGJ}  jx(ip_IO); {&2342}
<J82001>  HOI     + hv = I + OH               : {%TrGJ}  jx(ip_HOI); {&2342}
<J83001>  INO2    + hv = I + NO2              : {%TrGJ}  jx(ip_INO2); {&2342}
<J83101>  INO3    + hv = I + NO3              : {%TrGJ}  jx(ip_INO3); {&2342}
<J84001>  CH2I2   + hv = 2 I + 2 HO2 + CO     : {%TrGJ}  jx(ip_CH2I2); {&2342}
<J84101>  CH3I    + hv = I + CH3              : {%TrGJ}  jx(ip_CH3I); {&2342}
<J84102>  C3H7I   + hv = 2 LCARBON + I + CH3  : {%TrGJ}  jx(ip_C3H7I); {&2342}
<J84103>  CH2ClI  + hv = I + Cl + 2 HO2 + CO  : {%TrGJ}  jx(ip_CH2ClI); {&2342}
<J86001>  ICl     + hv = I + Cl               : {%TrGJ}  jx(ip_ICl); {&2342}
<J87001>  IBr     + hv = I + Br               : {%TrGJ}  jx(ip_IBr); {&2342}
{<J9nnn> ------------------------------ S ------------------------}{@\myhline}
{<HETnnn> ----------------------------- HET ----------------------}{@\myhline}
<HET200> N2O5 + H2O  = 2 HNO3       : {%StHet} khet_St(ihs_N2O5_H2O); {&SGN}
<HET201> N2O5        = 2 NO3m_cs + 2 Hp_cs : {%TrHet} khet_Tr(iht_N2O5); {&SGN}
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<HET410> HOCl  + HCl = Cl2 + H2O    : {%StHet}   khet_St(ihs_HOCl_HCl); {&SGN}
<HET420> ClNO3 + HCl = Cl2 + HNO3   : {%StHet}   khet_St(ihs_ClNO3_HCl); {&SGN}
<HET421> ClNO3 + H2O = HOCl + HNO3  : {%StHet}   khet_St(ihs_ClNO3_H2O); {&SGN}
<HET422> N2O5  + HCl = ClNO2 + HNO3 : {%StHet}   khet_St(ihs_N2O5_HCl); {&SGN}
<HET510> HOBr  + HBr = Br2 + H2O    : {%StHet}   khet_St(ihs_HOBr_HBr); {&SGN}
<HET520> BrNO3 + H2O = HOBr + HNO3  : {%StHet}   khet_St(ihs_BrNO3_H2O); {&SGN}
<HET540> ClNO3 + HBr = BrCl + HNO3  : {%StHet}   khet_St(ihs_ClNO3_HBr); {&SGN}
<HET541> BrNO3 + HCl = BrCl + HNO3  : {%StHet}   khet_St(ihs_BrNO3_HCl); {&SGN}
<HET542> HOCl  + HBr = BrCl + H2O   : {%StHet}   khet_St(ihs_HOCl_HBr); {&SGN}
<HET543> HOBr  + HCl = BrCl + H2O   : {%StHet}   khet_St(ihs_HOBr_HCl); {&SGN}
<HET1001> Hg      = RGM_cs                        : {%StTrHet} khet_Tr(iht_Hg)  + khet_St(ihs_Hg); {&SGN}
<HET1002> HgO     = RGM_cs                        : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1003> HgCl    = RGM_cs + LCHLORINE            : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1004> HgCl2   = RGM_cs + 2 LCHLORINE          : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1005> HgBr    = RGM_cs + LBROMINE             : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1006> HgBr2   = RGM_cs + 2 LBROMINE           : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1007> ClHgBr  = RGM_cs + LCHLORINE + LBROMINE : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1008> BrHgOBr = RGM_cs + 2 LBROMINE           : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<HET1009> ClHgOBr = RGM_cs + LCHLORINE + LBROMINE : {%StTrHet} khet_Tr(iht_RGM) + khet_St(ihs_RGM); {&SGN}
<G9100>  SO + O2   = SO2 + O3P   : {%TrStGS} 1.25e-13*exp(-2190/temp); {&2626}
<G9101>  SO + O3   = SO2 + O2    : {%TrStGS} 3.4e-12*exp(-1100/temp); {&2626}
<G9102>  S  + O2   = SO  + O3P   : {%TrStGS} 2.3e-12; {&2626}
<G9201>  SH + O2   = OH  + SO    : {%TrStGS} 4.e-19; {&2626}
<G9202>  SO3 + H2O = H2SO4       : {%TrStGS} 8.5e-41*exp(6540./temp)*C(ind_H2O); {&&1555}
<G9406>  OCS + OH  = SH  + CO2   : {%TrStGS} 1.1e-13*exp(-1200./temp); {&2626}
<G9407>  OCS + O3P = CO  + SO    : {%TrStGS} 2.1e-11*exp(-2200./temp); {&2626}
<J9000>  OCS + hv  = CO  + S     : {%TrStGSJ} JX(ip_OCS); {&&}
<J9001>  SO2 + hv  = SO  + O3P   : {%TrStGSJ} 60.*JX(ip_OCS); {&&}
<J9002>  SO3 + hv   = SO2 + O3P  : {%TrStGSJ} JX(ip_SO3); {&&}
<J9003>  H2SO4 + hv = SO3 + H2O  : {%TrStGSJ} JX(ip_H2SO4); {&&}
{***** END:   gas-phase chemistry from gas_mom.eqn *****}
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