Experiments at FORD: Model including deuterated species

Model run using upper limit on CH3ONO impurity in CH2DONO of 0.00016, and updated rates from NIST, IUPAC, JPL.

General description and conditions

Model of photochemistry of CH2DO + O2 forming CH2O vs CHDO
Experiments with CH2DONO precursor in the FORD photochemical reactor
Modeling series starting 02-21-18

> restart;
> ppm := 1e-6: ppb := 1e-9: ppt := 1e-12:
> T:= 273 + 23:
Ptot := 700:
> P:= 101300*Ptot/760:

Chemical equations

1a. $CH3ONO + hv \longrightarrow CH3O + NO$
1b. $CH2DONO + hv \longrightarrow CH2DO + NO$
2a. $CH3O + O2 \longrightarrow CH2O + HO2$
2b. $CH2DO + O2 \longrightarrow CH2O + DO2$
2c. $CH2DO + O2 \longrightarrow CHDO + HO2$
3a. $HO2 + NO \longrightarrow OH + NO2$
3b. $DO2 + NO \longrightarrow OD + NO2$
4a. $OH + cC6H12 \longrightarrow H2O + RO2$
4b. $OD + cC6H12 \longrightarrow HDO + RO2$
5. $RO2 + NO \longrightarrow RO + NO2$
6. $NO2 + hv \longrightarrow NO + O$
7. $O + O2 + M \longrightarrow O3 + M$
8a. $CH2O + hv \longrightarrow CO + H2$
8b. $CHDO + hv \longrightarrow CO + HD$
9a. $CH2O + hv \longrightarrow CO + 2*HO2$
9b. $CHDO + hv \longrightarrow CO + HO2 + DO2$
10a. $HO2 + NO2 + M \longrightarrow PNA + M$
10b. $DO2 + NO2 + M \longrightarrow PNAD + M$
11a. $HO2 + CH2O \longrightarrow HOCH2O2$
11b. $DO2 + CH2O \longrightarrow DOCH2O2$
11c. $HO2 + CHDO \longrightarrow HOCHDO2$
11d. $DO2 + CHDO \longrightarrow DOCHDO2$
12a. $HOCH2O2 + RO2 \longrightarrow HCOOH + RO + HO2$
12b. $DOCH2O2 + RO2 \longrightarrow HCOOD + RO + HO2$
12c. $HOCHDO2 + RO2 \longrightarrow DCOOH + RO + HO2$
12d. $DOCHDO2 + RO2 \longrightarrow DCOOD + RO + HO2$
13a. $CH3O + NO + M \longrightarrow CH3ONO + M$
13b. $CH2DO + NO + M \longrightarrow CH2DONO + M$
14a. $CH3O + NO2 + M \longrightarrow CH3ONO2 + M$
14b. $CH2DO + NO2 + M \longrightarrow CH2DONO2 + M$
15a. $OH + CH3ONO \longrightarrow CH2O + NO + H2O$
15b. $OH + CH2DONO \longrightarrow CHDO + NO + H2O$

15c. OH + CH2DONO --> CH2O + NO + HDO
15d. OD + CH2DONO --> CH2O + NO + D2O
15e. OD + CH2DONO --> CHDO + NO + HDO
15f. OD + CH3ONO --> CH2O + NO + HDO
16a. CH2O + OH --> H2O + CO + HO2
16b. CHDO + OH --> H2O + CO + DO2
16c. CHDO + OH --> HDO + CO + HO2
16d. CHDO + OD --> D2O + CO + HO2
16e. CHDO + OD --> HDO + CO + DO2
16f. CH2O + OD --> HDO + CO + HO2
17a. HO2 + HO2 --> H2O2
17b. HO2 + DO2 --> HDO2
17c. DO2 + DO2 --> D2O2
18a. H2O2 + *hv* --> 2OH
18b. HDO2 + *hv* --> OH + OD
18c. D2O2 + *hv* --> 2OD
19a. CH3O + NO2 --> CH2O + HONO
19b. CH2DO + NO2 --> CHDO + HONO
19c. CH2DO + NO2 --> CH2O + DONO
20a. HOCH2O2 + HOCH2O2 + O2 --> 2HCOOH + 2HO2
20b. HOCH2O2 + HOCHDO2 + O2 --> 1.5HCOOH + 0.5DCOOH + 1.5HO2 + 0.5DO2
20c. HOCH2O2 + DOCH2O2 + O2 --> HCOOH + HCOOD + 2HO2
20d. HOCH2O2 + DOCHDO2 + O2 --> HCOOH + 0.5HCOOD + 0.5DCOOD + 1.5HO2 + 0.5DO2
20e. HOCHDO2 + HOCH2O2 + O2 --> 0.5DCOOH + 1.5HCOOH + 1.5HO2 + 0.5DO2
20f. HOCHDO2 + HOCHDO2 + O2 --> DCOOH + HCOOH + HO2 + DO2
20g. HOCHDO2 + DOCH2O2 + O2 --> 0.5DCOOH + HCOOD + 0.5HCOOH + 1.5HO2 + 0.5DO2
20h. HOCHDO2 + DOCHDO2 + O2 --> 0.5DCOOH + 0.5HCOOH + 0.5HCOOD + 0.5DCOOD + HO2 + DO2
20i. DOCH2O2 + HOCH2O2 + O2 --> HCOOD + HCOOH + 2HO2
20j. DOCH2O2 + HOCHDO2 + O2 --> HCOOD + 0.5HCOOH + 0.5DCOOH + 1.5HO2 + 0.5DO2
20k. DOCH2O2 + DOCH2O2 +O2 --> 2HCOOD + 2HO2
20l. DOCH2O2 + DOCHDO2 + O2 --> 1.5HCOOD +0.5DCOOD + 1.5HO2 + 0.5DO2
20m. DOCHDO2 + HOCH2O2 + O2 --> 0.5DCOOD + 0.5HCOOD + HCOOH + 1.5HO2 + 0.5DO2
20n. DOCHDO2 + HOCHDO2 + O2 --> 0.5DCOOD + 0.5HCOOD + 0.5HCOOH + 0.5DCOOH + HO2 + DO2
20o. DOCHDO2 + DOCH2O2 + O2 --> 0.5DCOOD + 1.5HCOOD + 1.5HO2 + 0.5DO2
20p. DOCHDO2 + DOCHDO2 + O2 --> DCOOD + HCOOD + HO2 + DO2
21a. CH3OH + OH --> CH2OH + H2O
21b. CH2DOH + OH --> CH2OH + HDO
21c. CH2DOH + OH --> CHDOH + H2O
21d. CH3OH + OD --> CH2OH + HDO
21e. CH2DOH + OD --> CHDOH + HDO
21f. CH2DOH + OD --> CH2OH + D2O
22a. CH2OH + O2 --> CH2O + HO2
22b. CHDOH + O2 --> CHDO + HO2
23. O3 + NO --> NO2

24a. CO + OH --> CO2 + HO2
24b. CO + OD --> CO2 + DO2
25a. H2 + OH --> H2O + HO2
25b. HD + OH --> H2O + DO2
25c. HD + OH --> HDO + HO2
25d. H2 + OD --> HDO + HO2
25e. HD + OD -->HDO + DO2
25f. HD + OD -->D2O + HO2
26. RO2 + RO2 --> 2RO
27. RO2 + RO2 --> RO + cC6H12
28a. RO2 + HO2 --> cC6H12 (recycle)
28b. RO2 + DO2 --> cC6H12
29. RO + O2 --> cC6H12 + HO2
30aa. HOCH2O2 + HO2 --> HOCH2OOH + O2
30ab.   HOCH2O2 + DO2 --> HOCH2OOD + O2
30ac. DOCH2O2 + HO2 --> DOCH2OOH + O2
30ad. DOCH2O2 + DO2 --> DOCH2OOD + O2
30ae. HOCHDO2 + HO2 --> HOCHDOOH + O2
30af. HOCHDO2 + DO2 --> HOCHDOOD + O2
30ag. DOCHDO2 + HO2 --> HOCHDOOH + O2
30ah. DOCHDO2 + DO2 --> HOCHDOOD + O2
30ba. HOCH2O2 + HO2 --> HCOOH + H2O + O2
30bb.   HOCH2O2 + DO2 --> HCOOH + HDO + O2
30bc. DOCH2O2 + HO2 --> HCOOD + H2O + O2
30bd. DOCH2O2 + DO2 --> HCOOD + HDO + O2
30be. HOCHDO2 + HO2 --> DCOOH + H2O + O2
30bf. HOCHDO2 + DO2 --> DCOOH + HDO + O2
30bg. DOCHDO2 + HO2 --> DCOOD + H2O + O2
30bh. DOCHDO2 + DO2 --> DCOOD + HDO + O2
30ca. HOCH2O2 + HO2 --> HOCH2O + OH + O2
30cb.   HOCH2O2 + DO2 --> HOCH2O + OD + O2
30cc. DOCH2O2 + HO2 --> DOCH2O + OH + O2
30cd. DOCH2O2 + DO2 --> DOCH2O + OD + O2
30ce. HOCHDO2 + HO2 --> HOCHDO + OH + O2
30cf. HOCHDO2 + DO2 --> HOCHDO + OD + O2
30cg. DOCHDO2 + HO2 --> HOCHDO + OH + O2
30ch. DOCHDO2 + DO2 --> DOCHDO + OD + O2
31a. NO2 + OH + M --> HNO3
31b. NO2 + OD + M --> DNO3
32a. CH3ONO2 + OH --> CH2O + H2O + NO2
32b. CH2DONO2 + OH --> CH2O + HDO + NO2
32c. CH2DONO2 + OH --> CHDO + H2O + NO2
32d. CH3ONO2 + OD --> CH2O + HDO + NO2
32e. CH2DONO2 + OD --> CH2O + D2O + NO2
32f. CH2DONO2 + OD --> CHDO + HDO + NO2
33a. HOCH2O2 --> HO2 + CH2O
33b. DOCH2O2 --> DO2 + CH2O
33c. HOCHDO2 --> HO2 + CHDO
33d. DOCHDO2 --> DO2 + CHDO

Parameters

Time unit in the calculations
```
> time_unit:= second:
```
Number of time steps in the calculations
```
> nrt:= 300:
> time_tot:= time_unit*nrt:
```

Fundamental constants

Physical constants are present in Maple after the call:
with(ScientificConstants):
Avogadros number
```
> Na:= evalf(Constant(N[A])):
```
The gas contant
```
> R:= evalf(Constant(R)):
```

Fixed concentrations and Rate constants

Concentrations
Number of molecules per cm3 is calculated from temperature and pressure

$$M_i := \frac{P_i \, 10^{(-6)} \, Na}{R \, T_i}$$

Torr is defined in units of molecules per cc.

$$> \quad M := \frac{1}{1000000} \frac{P \, Na}{R \, T}; \; 1; \; Torr := \frac{1}{760} M; \; 1$$

$$M := 2.283066164 \, 10^{19}$$

$$1$$

$$Torr := 3.004034426 \, 10^{16}$$

$$1$$

Fixed concentrations
```
> O2:= 100*Torr:
N2 := 600*Torr:
> iso_impurity:=0.00016:#upper limit on CH3 contamination in
CH2DONO/CH2DOH from IR spectra.
```
Initial concentrations of time-varying species, modeling series starting 02-21-18
```
> CH3ONO_zero := iso_impurity*36.8*Torr/1000:
> CH2DONO_zero := (1-iso_impurity)*36.8*Torr/1000:
> CH3OH_zero := iso_impurity*1.48*Torr/1000:
> CH2DOH_zero := (1-iso_impurity)*1.48*Torr/1000:
> C6H12_zero := 75.3*Torr/1000:
```

```
> NO2_zero := 0:
> startconc := 0:
```
The rate constants:

1a. $CH3ONO + h\nu \rightarrow CH3O + NO$
```
> j1a:=1.44e-3: R1a:=j1a*CH3ONO(t):
```
1b. $CH2DONO + h\nu \rightarrow CH2DO + NO$
```
> j1b:=1.44e-3: R1b:=j1a*CH2DONO(t):
```
The rates $j1a$ and $j1b$ are set to be equal since deuteration has little effect on the chromophore.

2a. $CH3O + O2 \rightarrow CH2O + HO2$
```
> k2a:= 1.9e-15: R2a:=k2a*CH3O(t)*O2:
```
2b. $CH2DO + O2 \rightarrow CH2O + DO2$
```
> k2b:= (1/7.593)*(2/3)*1.9e-15: R2b:=k2b*CH2DO(t)*O2:
```
2c. $CH2DO + O2 \rightarrow CHDO + HO2$
```
> k2c:= (2/3)*1.9e-15: R2c:=k2c*CH2DO(t)*O2:
```
The rate $k2c$ is 2/3 that of $k2a$ because there are two hydrogen atoms, not three. The rate $k2b$ is (1/7.593)*(2/3) to match the first-order experimental result.

3a. $HO2 + NO \rightarrow OH + NO2$
```
> k3a:= 8.1e-12: R3a:=k3a*HO2(t)*NO(t):
```
3b. $DO2 + NO \rightarrow OD + NO2$
```
> k3b:= 8.1e-12: R3b:=k3b*DO2(t)*NO(t):
```
4a. $OH + cC6H12 \rightarrow H2O + RO2$
```
> k4a := 6.7e-12: R4a:=k4a*OH(t)*C6H12(t):
```
4b. $OD + cC6H12 \rightarrow HDO + RO2$
```
> k4b := k4a: R4b:=k4b*OD(t)*C6H12(t):
```
5. $RO2 + NO \rightarrow RO + NO2$
```
> k5 := 3e-12: R5:=k5*RO2(t)*NO(t):
```
6. $NO2 + h\nu \rightarrow NO + O$
```
> j6 := 2*j1a: R6:=j6*NO2(t):
```
7. $O + O2 + M \rightarrow O3 + M$
```
> k7 := 6.1e-34: R7:=k7*O_atom(t)*O2*M:
```
8. Formaldehyde photolysis with the Ford chamber lamps is about 0.05 % as fast as that of methyl nitrite. It will be divided 1:3 between radical and molecular channels. The relative photolysis rates for the deuterated formaldehydes, channel specific, are taken from Feilberg et al., 2007: molecular jhcho/jhcdo = 1.82; radical jhcho/jhcdo = 1.10

8a. $CH2O + h\nu \rightarrow CO + H2$
```
> j8a := 0.05*0.75*j1a: R8a:=j8a*CH2O(t):
```
8b. $CHDO + h\nu \rightarrow CO + HD$
```
> j8b := j8a/1.82: R8b:=j8b*CHDO(t):
```
9a. $CH2O + h\nu \rightarrow CO + 2*HO2$
```
> j9a := 0.05*0.25*j1a: R9a:=j9a*CH2O(t):
```
9b. $CHDO + h\nu \rightarrow CO + HO2 + DO2$
```
> j9b := j9a/1.10: R9b:=j9b*CHDO(t):
```
10a. $HO2 + NO2 + M \rightarrow PNA + M$
```
> k10a := 1.8e-31: R10a:=k10a*HO2(t)*NO2(t)*M:
```
10b. $DO2 + NO2 + M \rightarrow PNAD + M$
```
> k10b := 1.8e-31: R10b:=k10b*DO2(t)*NO2(t)*M:
```
11a. $HO2 + CH2O \rightarrow HOCH2O2$
```
> k11a := 8.01e-14: R11a:=k11a*HO2(t)*CH2O(t):
```
11b. $DO2 + CH2O \rightarrow DOCH2O2$

```
> k11b := 8.01e-14: R11b:=k11b*DO2(t)*CH2O(t):
```
11c. HO2 + CHDO --> HOCHDO2
```
> k11c := 8.01e-14: R11c:=k11c*HO2(t)*CHDO(t):
```
11d. DO2 + CHDO --> DOCHDO2
```
> k11d := 8.01e-14: R11d:=k11d*DO2(t)*CHDO(t):
```
12a. HOCH2O2 + RO2 --> HCOOH + RO + HO2
```
> k12a := 5e-14: R12a:=k12a*HOCH2O2(t)*RO2(t):
```
12b. DOCH2O2 + RO2 --> HCOOD + RO + HO2
```
> k12b := 5e-14: R12b:=k12b*DOCH2O2(t)*RO2(t):
```
12c. HOCHDO2 + RO2 --> DCOOH + RO + HO2
```
> k12c := 5e-14: R12c:=k12c*HOCHDO2(t)*RO2(t):
```
12d. DOCHDO2 + RO2 --> DCOOD + RO + HO2
```
> k12d := 5e-14: R12d:=k12d*DOCHDO2(t)*RO2(t):
```
13a. CH3O + NO + M --> CH3ONO + M
```
> k13a := 1.4e-29: R13a:=k13a*CH3O(t)*NO(t)*M:
```
13b. CH2DO + NO + M --> CH2DONO + M
```
> k13b := 1.4e-29: R13b:=k13b*CH2DO(t)*NO(t)*M:
```
14a. CH3O + NO2 + M --> CH3ONO2 + M
```
> k14a := 5.3e-29: R14a:=k14a*CH3O(t)*NO2(t)*M:
```
14b. CH2DO + NO2 + M --> CH2DONO2 + M
```
> k14b := 5.3e-29: R14b:=k14b*CH2DO(t)*NO2(t)*M:
```
15a. OH + CH3ONO --> CH2O + NO + H2O
```
> k15a := 3.0e-13: R15a:=k15a*OH(t)*CH3ONO(t):
```
15b. OH + CH2DONO --> CHDO + NO + H2O
```
> k15b := (2/3)*k15a: R15b:=k15b*OH(t)*CH2DONO(t):
```
15c. OH + CH2DONO --> CH2O + NO + HDO, factor of 1/8 based on relative reactivity of CD in methane.
```
> k15c := (1/3)*(1/8)*k15a: R15c:=k15c*OH(t)*CH2DONO(t):
```
15d. OD + CH2DONO --> CH2O + NO + D2O
```
> k15d := (1/3)*(1/8)*k15a: R15d:=k15d*OD(t)*CH2DONO(t):
```
15e. OD + CH2DONO --> CHDO + NO + HDO
```
> k15e := (2/3)*k15a: R15e:=k15e*OD(t)*CH2DONO(t):
```
15f. OD + CH3ONO --> CH2O + NO + HDO
```
> k15f := k15a: R15f:=k15f*OD(t)*CH3ONO(t):
```
16a. CH2O + OH --> H2O + CO + HO2
```
> k16a := 8.5e-12: R16a:=k16a*CH2O(t)*OH(t):
```
16b. CHDO + OH --> H2O + CO + DO2, from Feilberg 2004, k(OH+HCHO/kOH+HCDO) 1.28
```
> k16b := (8/9)*k16a/1.28: R16b:=k16b*CHDO(t)*OH(t):
```
16c. CHDO + OH --> HDO + CO + HO2
```
> k16c := (1/9)*k16a/1.28: R16c:=k16c*CHDO(t)*OH(t):
```
16d. CHDO + OD --> D2O + CO + HO2
```
> k16d := (1/9)*k16a/1.28: R16d:=k16d*CHDO(t)*OD(t):
```
16e. CHDO + OD --> HDO + CO + DO2
```
> k16e := (8/9)*k16a/1.28: R16e:=k16e*CHDO(t)*OD(t):
```
16f. CH2O + OD --> HDO + CO + HO2
```
> k16f := k16a: R16f:=k16f*CH2O(t)*OD(t):
```
17a. HO2 + HO2 --> H2O2
```
> k17a := 1.7e-12: R17a:=k17a*HO2(t)*HO2(t):
```
17b. HO2 + DO2 --> HDO2

```
> k17b := 8.6e-13: R17b:=k17b*HO2(t)*DO2(t):
```
17c. DO2 + DO2 --> D2O2
```
> k17c := 2.0e-14: R17c:=k17c*DO2(t)*DO2(t):
```
18a. H2O2 + *hv* --> 2OH, the photolysis rates are 0.0038 that of methyl nitrite
```
> j18a:=0.0038*j1a: R18a:=j18a*H2O2(t):
```
18b. HDO2 + *hv* --> OH + OD
```
> j18b:=0.0038*j1a: R18b:=j18b*HDO2(t):
```
18c. D2O2 + *hv* --> 2OD
```
> j18c:=0.0038*j1a: R18c:=j18c*D2O2(t):
```
19a. CH3O + NO2 --> CH2O + HONO
```
> k19a := 2.0e-13: R19a:=k19a*CH3O(t)*NO2(t):
```
19b. CH2DO + NO2 --> CHDO + HONO
```
> k19b := (2/3)*k19a: R19b:=k19b*CH2DO(t)*NO2(t):
```
19c. CH2DO + NO2 --> CH2O + DONO
```
> k19c := (1/8)*(1/3)*k19a: R19c:=k19c*CH2DO(t)*NO2(t):
```
20a. HOCH2O2 + HOCH2O2 + O2 --> 2HCOOH + 2HO2
```
> k20a := 5.5e-12: R20a:=k20a*HOCH2O2(t)*HOCH2O2(t)*O2(t):
```
20b. HOCH2O2 + HOCHDO2 + O2 --> 1.5HCOOH + 0.5DCOOH + 1.5HO2 + 0.5DO2
```
> k20b := 5.5e-12: R20b:=k20b*HOCH2O2(t)*HOCHDO2(t)*O2(t):
```
20c. HOCH2O2 + DOCH2O2 + O2 --> HCOOH + HCOOD + 2HO2
```
> k20c := 5.5e-12: R20c:=k20c*HOCH2O2(t)*DOCH2O2(t)*O2(t):
```
20d. HOCH2O2 + DOCHDO2 + O2 --> HCOOH + 0.5HCOOD + 0.5DCOOD + 1.5HO2 + 0.5DO2
```
> k20d := 5.5e-12: R20d:=k20d*HOCH2O2(t)*DOCHDO2(t)*O2(t):
```
20e. HOCHDO2 + HOCH2O2 + O2 --> 0.5DCOOH + 1.5HCOOH + 1.5HO2 + 0.5DO2
```
> k20e := 5.5e-12: R20e:=k20e*HOCHDO2(t)*HOCH2O2(t)*O2(t):
```
20f. HOCHDO2 + HOCHDO2 + O2 --> DCOOH + HCOOH + HO2 + DO2
```
> k20f := 5.5e-12: R20f:=k20f*HOCHDO2(t)*HOCHDO2(t)*O2(t):
```
20g. HOCHDO2 + DOCH2O2 + O2 --> 0.5DCOOH + HCOOD + 0.5HCOOH + 1.5HO2 + 0.5DO2
```
> k20g := 5.5e-12: R20g:=k20g*HOCHDO2(t)*DOCH2O2(t)*O2(t):
```
20h. HOCHDO2 + DOCHDO2 + O2 --> 0.5DCOOH + 0.5HCOOH + 0.5HCOOD + 0.5DCOOD + HO2 + DO2
```
> k20h := 5.5e-12: R20h:=k20h*HOCHDO2(t)*DOCHDO2(t)*O2(t):
```
20i. DOCH2O2 + HOCH2O2 + O2 --> HCOOD + HCOOH + 2HO2
```
> k20i := 5.5e-12: R20i:=k20i*DOCH2O2(t)*HOCH2O2(t)*O2(t):
```
20j. DOCH2O2 + HOCHDO2 + O2 --> HCOOD + 0.5HCOOH + 0.5DCOOH + 1.5HO2 + 0.5DO2
```
> k20j := 5.5e-12: R20j:=k20j*DOCH2O2(t)*HOCHDO2(t)*O2(t):
```
20k. DOCH2O2 + DOCH2O2 +O2 --> 2HCOOD + 2HO2
```
> k20k := 5.5e-12: R20k:=k20k*DOCH2O2(t)*DOCH2O2(t)*O2(t):
```
20l. DOCH2O2 + DOCHDO2 + O2 --> 1.5HCOOD +0.5DCOOD + 1.5HO2 + 0.5DO2
```
> k20l := 5.5e-12: R20l:=k20l*DOCH2O2(t)*DOCHDO2(t)*O2(t):
```
20m. DOCHDO2 + HOCH2O2 + O2 --> 0.5DCOOD + 0.5HCOOD + HCOOH + 1.5HO2 + 0.5DO2
```
> k20m := 5.5e-12: R20m:=k20m*DOCHDO2(t)*HOCH2O2(t)*O2(t):
```
20n. DOCHDO2 + HOCHDO2 + O2 --> 0.5DCOOD + 0.5HCOOD + 0.5HCOOH + 0.5DCOOH + HO2 + DO2
```
> k20n := 5.5e-12: R20n:=k20n*DOCHDO2(t)*HOCHDO2(t)*O2(t):
```
20o. DOCHDO2 + DOCH2O2 + O2 --> 0.5DCOOD + 1.5HCOOD + 1.5HO2 + 0.5DO2

> **k20o := 5.5e-12: R20o:=k20o*DOCHDO2(t)*DOCH2O2(t)*O2(t):**

20p. $DOCHDO2 + DOCHDO2 + O2 \longrightarrow DCOOD + HCOOD + HO2 + DO2$

> **k20p := 5.5e-12: R20p:=k20p*DOCHDO2(t)*DOCHDO2(t)*O2(t):**

21a. $CH3OH + OH \longrightarrow CH2OH + H2O$

k21a := 8.8e-13: R21a:=k21a*CH3OH(t)*OH(t):

21b. $CH2DOH + OH \longrightarrow CH2OH + HDO$

> **k21b := (1/3)*(1/8)*k21a: R21b:=k21b*CH2DOH(t)*OH(t):**

21c. $CH2DOH + OH \longrightarrow CHDOH + H2O$

> **k21c := (2/3)*k21a: R21c:=k21c*CH2DOH(t)*OH(t):**

21d. $CH3OH + OD \longrightarrow CH2OH + HDO$

> **k21d := k21a: R21d:=k21d*CH3OH(t)*OD(t):**

21e. $CH2DOH + OD \longrightarrow CHDOH + HDO$

> **k21e := (2/3)*k21a: R21e:=k21e*CH2DOH(t)*OD(t):**

21f. $CH2DOH + OD \longrightarrow CH2OH + D2O$

> **k21f := (1/3)*(1/8)*k21a: R21f:=k21f*CH2DOH(t)*OD(t):**

22a. $CH2OH + O2 \longrightarrow CH2O + HO2$

> **k22a := 9.6e-12: R22a:=k22a*CH2OH(t)*O2:**

22b. $CHDOH + O2 \longrightarrow CHDO + HO2$

> **k22b := 9.6e-12: R22b:=k22b*CHDOH(t)*O2:**

23. $O3 + NO \longrightarrow NO2$

> **k23 := 1.9e-14: R23:=k23*O3(t)*NO(t):**

24a. $CO + OH \longrightarrow CO2 + HO2$

> **k24a := 2.3e-13: R24a:=k24a*CO(t)*OH(t):**

24b. $CO + OD \longrightarrow CO2 + DO2$

> **k24b := 5.0e-14: R24b:=k24b*CO(t)*OD(t):**

25a. $H2 + OH \longrightarrow H2O + HO2$

> **k25a := 6.7e-15: R25a:=k25a*H2(t)*OH(t):**

25b. $HD + OH \longrightarrow H2O + DO2$

> **k25b := 2.5e-15: R25b:=k25b*HD(t)*OH(t):**

25c. $HD + OH \longrightarrow HDO + HO2$

> **k25c := 6.7e-16: R25c:=k25c*HD(t)*OH(t):**

25d. $H2 + OD \longrightarrow HDO + HO2$

> **k25d := 7.4e-15: R25d:=k25d*H2(t)*OD(t):**

25e. $HD + OD \longrightarrow HDO + DO2$

> **k25e := 0.9*k25b: R25e:=k25e*HD(t)*OD(t):**

25f. $HD + OD \longrightarrow D2O + HO2$

> **k25f := 0.9*k25c: R25f:=k25f*HD(t)*OD(t):**

26. $RO2 + RO2 \longrightarrow 2RO$

> **k26 := 8.2e-15: R26:=k26*RO2(t)*RO2(t):**

27. $RO2 + RO2 \longrightarrow RO + cC6H12$

> **k27 := 2.0e-14: R27:=k27*RO2(t)*RO2(t):**

28a. $RO2 + HO2 \longrightarrow cC6H12$

> **k28a := 3.5e-11: R28a:=k28a*RO2(t)*HO2(t):**

28b. $RO2 + DO2 \longrightarrow cC6H12$

> **k28b := k28a: R28b:=k28b*RO2(t)*DO2(t):**

29. $RO + O2 \longrightarrow cC6H12 + HO2$

> **k29 := 2.0e-17: R29:=k29*RO(t)*O2:**

30aa. $HOCH2O2 + HO2 \longrightarrow HOCH2OOH + O2$

> **k30aa := 6.0e-12: R30aa:=k30aa*HOCH2O2(t)*HO2(t):**

30ab. $HOCH2O2 + DO2 \longrightarrow HOCH2OOD + O2$

```
> k30ab := k30aa: R30ab:=k30ab*HOCH2O2(t)*DO2(t):
```
30ac. DOCH2O2 + HO2 --> DOCH2OOH + O2
```
> k30ac := k30aa: R30ac:=k30ac*DOCH2O2(t)*HO2(t):
```
30ad. DOCH2O2 + DO2 --> DOCH2OOD + O2
```
> k30ad := k30aa: R30ad:=k30ad*DOCH2O2(t)*DO2(t):
```
30ae. HOCHDO2 + HO2 --> HOCHDOOH + O2
```
> k30ae := k30aa: R30ae:=k30ae*HOCHDO2(t)*HO2(t):
```
30af. HOCHDO2 + DO2 --> HOCHDOOD + O2
```
> k30af := k30aa: R30af:=k30af*HOCHDO2(t)*DO2(t):
```
30ag. DOCHDO2 + HO2 --> HOCHDOOH + O2
```
> k30ag := k30aa: R30ag:=k30ag*DOCHDO2(t)*HO2(t):
```
30ah. DOCHDO2 + DO2 --> HOCHDOOD + O2
```
> k30ah := k30aa: R30ah:=k30ah*DOCHDO2(t)*DO2(t):
```
30ba. HOCH2O2 + HO2 --> HCOOH + H2O + O2
```
> k30ba := 3.6e-12: R30ba:=k30ba*HOCH2O2(t)*HO2(t):
```
30bb. HOCH2O2 + DO2 --> HCOOH + HDO + O2
```
> k30bb := k30ba: R30bb:=k30bb*HOCH2O2(t)*DO2(t):
```
30bc. DOCH2O2 + HO2 --> HCOOD + H2O + O2
```
> k30bc := k30ba: R30bc:=k30bc*DOCH2O2(t)*HO2(t):
```
30bd. DOCH2O2 + DO2 --> HCOOD + HDO + O2
```
> k30bd := k30ba: R30bd:=k30bd*DOCH2O2(t)*DO2(t):
```
30be. HOCHDO2 + HO2 --> DCOOH + H2O + O2
```
> k30be := k30ba: R30be:=k30be*HOCHDO2(t)*HO2(t):
```
30bf. HOCHDO2 + DO2 --> DCOOH + HDO + O2
```
> k30bf := k30ba: R30bf:=k30bf*HOCHDO2(t)*DO2(t):
```
30bg. DOCHDO2 + HO2 --> DCOOD + H2O + O2
```
> k30bg := k30ba: R30bg:=k30bg*DOCHDO2(t)*HO2(t):
```
30bh. DOCHDO2 + DO2 --> DCOOD + HDO + O2
```
> k30bh := k30ba: R30bh:=k30bh*DOCHDO2(t)*DO2(t):
```
30ca. HOCH2O2 + HO2 --> HOCH2O + OH + O2
```
> k30ca := 2.4e-12: R30ca:=k30ca*HOCH2O2(t)*HO2(t):
```
30cb. HOCH2O2 + DO2 --> HOCH2O + OD + O2
```
> k30cb := k30ca: R30cb:=k30cb*HOCH2O2(t)*DO2(t):
```
30cc. DOCH2O2 + HO2 --> DOCH2O + OH + O2
```
> k30cc := k30ca: R30cc:=k30cc*DOCH2O2(t)*HO2(t):
```
30cd. DOCH2O2 + DO2 --> DOCH2O + OD + O2
```
> k30cd := k30ca: R30cd:=k30cd*DOCH2O2(t)*DO2(t):
```
30ce. HOCHDO2 + HO2 --> HOCHDO + OH + O2
```
> k30ce := k30ca: R30ce:=k30ce*HOCHDO2(t)*HO2(t):
```
30cf. HOCHDO2 + DO2 --> HOCHDO + OD + O2
```
> k30cf := k30ca: R30cf:=k30cf*HOCHDO2(t)*DO2(t):
```
30cg. DOCHDO2 + HO2 --> HOCHDO + OH + O2
```
> k30cg := k30ca: R30cg:=k30cg*DOCHDO2(t)*HO2(t):
```
30ch. DOCHDO2 + DO2 --> DOCHDO + OD + O2
```
> k30ch := k30ca: R30ch:=k30ch*DOCHDO2(t)*DO2(t):
```
31a. NO2 + OH + M --> HNO3
```
> k31a := 4.1E-11:R31a := k31a*NO2(t)*OH(t):#M is included in rate,
cf JPL
```
31b. NO2 + OD + M --> DNO3
```
> k31b := 9.3E-11:R31b := k31b*NO2(t)*OD(t):
```

32a. CH3ONO2 + OH --> CH2O + H2O + NO2
```
> k32a := 3.0e-13: R32a:=k32a*OH(t)*CH3ONO2(t):
```
32b. CH2DONO2 + OH --> CH2O + HDO + NO2
```
> k32b := (1/3)*(1/8)*k32a: R32b:=k32b*OH(t)*CH2DONO2(t):
```
32c. CH2DONO2 + OH --> CHDO + H2O + NO2
```
> k32c := (2/3)*k32a: R32c:=k32c*OH(t)*CH2DONO2(t):
```
32d. CH3ONO2 + OD --> CH2O + HDO + NO2
```
> k32d := k32a: R32d:=k32d*OD(t)*CH3ONO2(t):
```
32e. CH2DONO2 + OD --> CH2O + D2O + NO2
```
> k32e := (1/3)*(1/8)*k32a: R32e:=k32e*OD(t)*CH2DONO2(t):
```
32f. CH2DONO2 + OD --> CHDO + HDO + NO2
```
> k32f := (2/3)*k32a: R32f:=k32f*OD(t)*CH2DONO2(t):
```
33a. HOCH2O2 --> HO2 + CH2O
```
> k33a := 150:R33a := k33a*HOCH2O2(t):
```
33b. DOCH2O2 --> DO2 + CH2O
```
> k33b := 150:R33b := k33b*DOCH2O2(t):
```
33c. HOCHDO2 --> HO2 + CHDO
```
> k33c := 150:R33c := k33c*HOCHDO2(t):
```
33d. DOCHDO2 --> DO2 + CHDO
```
> k33d := 150:R33d := k33d*DOCHDO2(t):
```

REFERENCES: Photolysis rate for CH3ONO is derived from experimental data, other photolysis rates calculated using estimated lamp flux curve and JPL cross section to derive a photolysis rate relative to methyl nitrite. Reaction rates are from JPL or NIST.

Definition of differential equations with initial conditions

For example the equation d(CH3ONO)/dt = -R1a+R13a-R15a-R15f is written:
```
> D_CH3ONO:= diff(CH3ONO(t),t) = -R1a+R13a-R15a-R15f,
CH3ONO(0)=CH3ONO_zero:
> D_CH3O:= diff(CH3O(t),t) = R1a - R2a - R13a - R14a - R19a,
CH3O(0)=startconc:
> D_NO:= diff(NO(t),t) =
R1a+R1b-R3a-R3b-R5+R6-R13a-R13b+R15a+R15b+R15c+R15d+R15e+R15f-
R23, NO(0) = startconc:
> D_CH2DONO:= diff(CH2DONO(t),t) = -R1b+R13b-R15b-R15c-R15d-R15e,
CH2DONO(0)=CH2DONO_zero:
> D_CH2DO:= diff(CH2DO(t),t) = R1b-R2b-R2c-R13b-R14b-R19b-R19c,
CH2DO(0)=startconc:
> D_CH2O:= diff(CH2O(t),t) =
R2a+R2b-R8a-R9a-R11a-R11b+R15a+R15c+R15d+R15f-R16a-R16f+R19a+R
19c+R22a+R32a+R32b+R32d+R32e+R33a+R33b, CH2O(0)=startconc:
> D_HO2:= diff(HO2(t),t) =
R2a+R2c-R3a+2*R9a+R9b-R10a-R11a-R11c+R12a+R12b+R12c+R12d+R16a+
R16c+R16d+R16f-2*R17a-R17b+2*R20a+1.5*R20b+2*R20c+1.5*R20d+1.5
*R20e+R20f+1.5*R20g+R20h+2*R20i+2*R20j+2*R20k+1.5*R20l+1.5*R20
m+R20n+1.5*R20o+R20p+R22a+R22b+R24a+R25a+R25c+R25d+R25f-R28a+R
29-R30aa-R30ac-R30ae-R30ag-R30ba-R30bc-R30be-R30bg-R30ca-R30cc
-R30ce-R30cg+R33a+R33c, HO2(0)=startconc:
```

```
> D_DO2:=diff(DO2(t),t) =
R2b-R3b+R9b-R10b-R11b-R11d+R16b+R16e-R17b-2*R17c+0.5*R20b+0.5*
R20d+0.5*R20e+0.5*R20f+0.5*R20g+0.5*R20h+0.5*R20j+0.5*R20l+0.5
*R20m+0.5*R20n+0.5*R20o+R20p+R24b+R25b+R25e-R28b-R30ab-R30ad-R
30af-R30ah-R30bb-R30bd-R30bf-R30bh-R30cb-R30cd-R30cf-R30ch+R33
b+R33d, DO2(0)=startconc:
> D_CHDO:=diff(CHDO(t),t) =
R2c-R8b-R9b-R11c-R11d+R15b+R15e-R16b-R16c-R16d-R16e+R19b+R22b+
R32c+R32f+R33c+R33d, CHDO(0)=startconc:
> D_OH:=diff(OH(t),t) =
R3a-R4a-R15a-R15b-R15c-R16a-R16b-R16c+2*R18a+R18b-R21a-R21b-R2
1c-R24a-R25a-R25b-R25c+R30ca+R30cc+R30ce+R30cg-R31a-R32a-R32b-
R32c, OH(0)=startconc:
> D_NO2:=diff(NO2(t),t) =
R3a+R3b+R5-R6-R10a-R10b-R14a-R14b-R19a-R19b-R19c+R23-R31a-R31b
+R32a+R32b+R32c+R32d+R32e+R32f, NO2(0)=NO2_zero:
> D_OD:=diff(OD(t),t) =
R3b-R4b-R15d-R15e-R15f-R16d-R16e-R16f+R18b+2*R18c-R21d-R21e-R2
1f-R24b-R25d-R25e-R25f+R30cb+R30cd+R30cf+R30ch-R31b-R32d-R32e-
R32f, OD(0)=startconc:
> D_C6H12:=diff(C6H12(t),t) = -R4a-R4b+R27+R28a+R28b+R29,
C6H12(0)=C6H12_zero:
> D_H2O:=diff(H2O(t),t) =
R4a+R15a+R15b+R16a+R16b+R21a+R21c+R25a+R25b+R30ba+R30bc+R30be+
R30bg+R32a+R32c, H2O(0)=startconc:
> D_RO2:=diff(RO2(t),t) =
R4a+R4b+R5-R12a-R12b-R12c-R12d-2*R26-2*R27-R28a-R28b,
RO2(0)=startconc:
> D_HDO:=diff(HDO(t),t) =
R4b+R15c+R15e+R15f+R16c+R16e+R16f+R21b+R21d+R21e+R25c+R25d+R25
e+R30bb+R30bd+R30bf+R30bh+R32b+R32d+R32f, HDO(0)=startconc:
> D_RO:=diff(RO(t),t) = R5+R12a+R12b+R12c+R12d+2*R26+R27-R29,
RO(0)=startconc:
> D_O_atom:=diff(O_atom(t),t) = R6-R7, O_atom(0)=startconc:
> D_O3:=diff(O3(t),t) = R7-R23, O3(0)=startconc:
> D_CO:=diff(CO(t),t) =
R8a+R8b+R9a+R9b+R16a+R16b+R16c+R16d+R16e+R16f-R24a-R24b,
CO(0)=startconc:
> D_H2:=diff(H2(t),t) = R8a-R25a-R25d, H2(0)=startconc:
> D_HD:=diff(HD(t),t) = R8b-R25b-R25c-R25f-R25e,
HD(0)=startconc:
> D_PNA:=diff(PNA(t),t) = R10a, PNA(0)=startconc:
> D_PNAD:=diff(PNAD(t),t) = R10b, PNAD(0)=startconc:
> D_HOCH2O2:=diff(HOCH2O2(t),t) =
R11a-R12a-R20d-R20e-R20i-R20m-R30aa-R30ab-R30ba-R30bb-R30ca-R3
0cb-R33a, HOCH2O2(0)=startconc:
> D_DOCH2O2:=diff(DOCH2O2(t),t) =
R11b-R12b-R20c-R20g-R20i-R20j-2*R20k-R20l-R20o-R30ac-R30ad-R30
bc-R30bd-R30cc-R30cd-R33b, DOCH2O2(0)=startconc:
> D_HOCHDO2:=diff(HOCHDO2(t),t) =
R11c-R12c-R20b-R20e-2*R20f-R20g-R20h-R20j-R20n-R30ae-R30af-R30
```

```
be-R30bf-R30ce-R30cf-R33c, HOCHDO2(0)=startconc:
> D_DOCHDO2:=diff(DOCHDO2(t),t) =
R11d-R12d-R20d-R20h-R20l-R20m-R20n-R20o-2*R20p-R30ag-R30ah-R30
bg-R30bh-R30cg-R30ch-R33d, DOCHDO2(0)=startconc:
> D_HCOOH:=diff(HCOOH(t),t) =
R12a+2*R20a+1.5*R20b+R20c+R20d+1.5*R20e+R20f+0.5*R20g+0.5*R20h
+R20i+0.5*R20j+R20m+0.5*R20n+R30ba+R30bb, HCOOH(0)=startconc:
> D_HCOOD:=diff(HCOOD(t),t) =
R12b+R20c+0.5*R20d+R20g+0.5*R20h+R20i+R20j+2*R20k+1.5*R20l+0.5
*R20m+0.5*R20n+1.5*R20o+R20p+R30bc+R30bd, HCOOD(0)=startconc:
> D_DCOOH:=diff(DCOOH(t),t) =
R12c+0.5*R20b+0.5*R20e+R20f+0.5*R20g+0.5*R20h+0.5*R20j+0.5*R20
n+R30be+R30bf, DCOOH(0)=startconc:
> D_DCOOD:=diff(DCOOD(t),t) =
R12d+0.5*R20d+0.5*R20h+0.5*R20l+0.5*R20m+0.5*R20n+0.5*R20o+R20
p+R30bg+R30bh, DCOOD(0)=startconc:
> D_CH3ONO2:=diff(CH3ONO2(t),t) = R14a-R32a-R32d,
CH3ONO2(0)=startconc:
> D_CH2DONO2:=diff(CH2DONO2(t),t) = R14b-R32b-R32c-R32e-R32f,
CH2DONO2(0)=startconc:
> D_D2O:=diff(D2O(t),t) = R15d+R16d+R21f+R25f+R32e,
D2O(0)=startconc:
> D_H2O2:=diff(H2O2(t),t) = R17a-R18a, H2O2(0)=startconc:
> D_HDO2:=diff(HDO2(t),t) = R17b-R18b, HDO2(0)=startconc:
> D_D2O2:=diff(D2O2(t),t) = R17c-R18c, D2O2(0)=startconc:
> D_HONO:=diff(HONO(t),t) = R19a+R19b, HONO(0)=startconc:
> D_DONO:=diff(DONO(t),t) = R19c, DONO(0)=startconc:
> D_CH2OHOH:=diff(CH2OHOH(t),t) = R20a+R20e+R20i+R20m,
CH2OHOH(0)=startconc:
> D_CHDOHOH:=diff(CHDOHOH(t),t) = R20b+R20f+R20j+R20n,
CHDOHOH(0)=startconc:
> D_CH2OHOD:=diff(CH2OHOD(t),t) = R20c+R20g+R20k+R20o,
CH2OHOD(0)=startconc:
> D_CHDOHOD:=diff(CHDOHOD(t),t) = R20d+R20h+R20l+R20p,
CHDOHOD(0)=startconc:
> D_CH3OH:=diff(CH3OH(t),t) = -R21a-R21d, CH3OH(0)=CH3OH_zero:
> D_CH2OH:=diff(CH2OH(t),t) = R21a+R21b+R21d+R21f-R22a,
CH2OH(0)=startconc:
> D_CH2DOH:=diff(CH2DOH(t),t) = R21b-R21c-R21e-R21f,
CH2DOH(0)=CH2DOH_zero:
> D_CHDOH:=diff(CHDOH(t),t) = R21c+R21e-R22b,
CHDOH(0)=startconc:
> D_CO2:=diff(CO2(t),t) = R24a+R24b, CO2(0)=startconc:
> D_HOCH2OOH:=diff(HOCH2OOH(t),t) = R30aa+R30ab,
HOCH2OOH(0)=startconc:
> D_DOCH2OOH:=diff(DOCH2OOH(t),t) = R30ac,
DOCH2OOH(0)=startconc:
> D_HOCHDOOH:=diff(HOCHDOOH(t),t) = R30ae+R30ag,
HOCHDOOH(0)=startconc:
> D_HOCHDOOD:=diff(HOCHDOOD(t),t) = R30af+R30ah,
HOCHDOOD(0)=startconc:
```

```
> D_DOCH2OOD:=diff(DOCH2OOD(t),t) = R30ad,
DOCH2OOD(0)=startconc:
> D_HOCH2O:=diff(HOCH2O(t),t) = R30ca+R30cb,
HOCH2O(0)=startconc:
> D_DOCH2O:=diff(DOCH2O(t),t) = R30cc+R30cd,
DOCH2O(0)=startconc:
> D_HOCHDO:=diff(HOCHDO(t),t) = R30ce+R30cf,
HOCHDO(0)=startconc:
> D_DOCHDO:=diff(DOCHDO(t),t) = R30cg+R30ch,
DOCHDO(0)=startconc:
> D_HNO3:=diff(HNO3(t),t) = R31a, HNO3(0)=startconc:
> D_DNO3:=diff(DNO3(t),t) = R31b, DNO3(0)=startconc:
```

The following are markers used in making budgets for species components.

```
> D_mR02a:=diff(mR02a(t),t) = R2a, mR02a(0) = startconc:
> D_mR02b:=diff(mR02b(t),t) = R2b, mR02b(0) = startconc:
> D_mR02c:=diff(mR02c(t),t) = R2c, mR02c(0) = startconc:
> D_mR03a:=diff(mR03a(t),t) = R3a, mR03a(0) = startconc:
> D_mR04a:=diff(mR04a(t),t) = R4a, mR04a(0) = startconc:
> D_mR08a:=diff(mR08a(t),t) = R8a, mR08a(0) = startconc:
> D_mR08b:=diff(mR08b(t),t) = R8b, mR08b(0) = startconc:
> D_mR09a:=diff(mR09a(t),t) = R9a, mR09a(0) = startconc:
> D_mR09b:=diff(mR09b(t),t) = R9b, mR09b(0) = startconc:
> D_mR10a:=diff(mR10a(t),t) = R10a, mR10a(0) = startconc:
> D_mR10b:=diff(mR10b(t),t) = R10b, mR10b(0) = startconc:
> D_mR11a:=diff(mR11a(t),t) = R11a, mR11a(0) = startconc:
> D_mR11b:=diff(mR11b(t),t) = R11b, mR11b(0) = startconc:
> D_mR11c:=diff(mR11c(t),t) = R11c, mR11c(0) = startconc:
> D_mR11d:=diff(mR11d(t),t) = R11d, mR11d(0) = startconc:
> D_mR12a:=diff(mR12a(t),t) = R12a, mR12a(0) = startconc:
> D_mR12b:=diff(mR12b(t),t) = R12b, mR12b(0) = startconc:
> D_mR12c:=diff(mR12c(t),t) = R12c, mR12c(0) = startconc:
> D_mR12d:=diff(mR12d(t),t) = R12d, mR12d(0) = startconc:
> D_mR15a:=diff(mR15a(t),t) = R15a, mR15a(0) = startconc:
> D_mR15b:=diff(mR15b(t),t) = R15b, mR15b(0) = startconc:
> D_mR15c:=diff(mR15c(t),t) = R15c, mR15c(0) = startconc:
> D_mR15d:=diff(mR15d(t),t) = R15d, mR15d(0) = startconc:
> D_mR15e:=diff(mR15e(t),t) = R15e, mR15e(0) = startconc:
> D_mR15f:=diff(mR15f(t),t) = R15f, mR15f(0) = startconc:
> D_mR16a:=diff(mR16a(t),t) = R16a, mR16a(0) = startconc:
> D_mR16b:=diff(mR16b(t),t) = R16b, mR16b(0) = startconc:
> D_mR16c:=diff(mR16c(t),t) = R16c, mR16c(0) = startconc:
> D_mR16d:=diff(mR16d(t),t) = R16d, mR16d(0) = startconc:
> D_mR16e:=diff(mR16e(t),t) = R16e, mR16e(0) = startconc:
> D_mR16f:=diff(mR16f(t),t) = R16f, mR16f(0) = startconc:
> D_mR17a:=diff(mR17a(t),t) = R17a, mR17a(0) = startconc:
> D_mR17b:=diff(mR17b(t),t) = R17b, mR17b(0) = startconc:
> D_mR17c:=diff(mR17c(t),t) = R17c, mR17c(0) = startconc:
> D_mR18a:=diff(mR18a(t),t) = R18a, mR18a(0) = startconc:
> D_mR18b:=diff(mR18b(t),t) = R18b, mR18b(0) = startconc:
> D_mR19a:=diff(mR19a(t),t) = R19a, mR19a(0) = startconc:
```

```
> D_mR19b:=diff(mR19b(t),t) = R19b, mR19b(0) = startconc:
> D_mR19c:=diff(mR19c(t),t) = R19c, mR19c(0) = startconc:
> D_mR20a:=diff(mR20a(t),t) = R20a, mR20a(0) = startconc:
> D_mR20b:=diff(mR20b(t),t) = R20b, mR20b(0) = startconc:
> D_mR20c:=diff(mR20c(t),t) = R20c, mR20c(0) = startconc:
> D_mR20d:=diff(mR20d(t),t) = R20d, mR20d(0) = startconc:
> D_mR20e:=diff(mR20e(t),t) = R20e, mR20e(0) = startconc:
> D_mR20f:=diff(mR20f(t),t) = R20f, mR20f(0) = startconc:
> D_mR20g:=diff(mR20g(t),t) = R20g, mR20g(0) = startconc:
> D_mR20h:=diff(mR20h(t),t) = R20h, mR20h(0) = startconc:
> D_mR20i:=diff(mR20i(t),t) = R20i, mR20i(0) = startconc:
> D_mR20j:=diff(mR20j(t),t) = R20j, mR20j(0) = startconc:
> D_mR20k:=diff(mR20k(t),t) = R20k, mR20k(0) = startconc:
> D_mR20l:=diff(mR20l(t),t) = R20l, mR20l(0) = startconc:
> D_mR20m:=diff(mR20m(t),t) = R20m, mR20m(0) = startconc:
> D_mR20n:=diff(mR20n(t),t) = R20n, mR20n(0) = startconc:
> D_mR20o:=diff(mR20o(t),t) = R20o, mR20o(0) = startconc:
> D_mR20p:=diff(mR20p(t),t) = R20p, mR20p(0) = startconc:
> D_mR21a:=diff(mR21a(t),t) = R21a, mR21a(0) = startconc:
> D_mR21b:=diff(mR21b(t),t) = R21b, mR21b(0) = startconc:
> D_mR21c:=diff(mR21c(t),t) = R21c, mR21c(0) = startconc:
> D_mR22a:=diff(mR22a(t),t) = R22a, mR22a(0) = startconc:
> D_mR22b:=diff(mR22b(t),t) = R22b, mR22b(0) = startconc:
> D_mR24a:=diff(mR24a(t),t) = R24a, mR24a(0) = startconc:
> D_mR25a:=diff(mR25a(t),t) = R25a, mR25a(0) = startconc:
> D_mR25b:=diff(mR25b(t),t) = R25b, mR25b(0) = startconc:
> D_mR25c:=diff(mR25c(t),t) = R25c, mR25c(0) = startconc:
> D_mR25d:=diff(mR25d(t),t) = R25d, mR25d(0) = startconc:
> D_mR25e:=diff(mR25e(t),t) = R25e, mR25e(0) = startconc:
> D_mR25f:=diff(mR25f(t),t) = R25f, mR25f(0) = startconc:
> D_mR28a:=diff(mR28a(t),t) = R28a, mR28a(0) = startconc:
> D_mR28b:=diff(mR28b(t),t) = R28b, mR28b(0) = startconc:
> D_mR29:=diff(mR29(t),t) = R29, mR29(0) = startconc:
> D_mR30aa:=diff(mR30aa(t),t) = R30aa, mR30aa(0) = startconc:
> D_mR30ab:=diff(mR30ab(t),t) = R30ab, mR30ab(0) = startconc:
> D_mR30ac:=diff(mR30ac(t),t) = R30ac, mR30ac(0) = startconc:
> D_mR30ad:=diff(mR30ad(t),t) = R30ad, mR30ad(0) = startconc:
> D_mR30ae:=diff(mR30ae(t),t) = R30ae, mR30ae(0) = startconc:
> D_mR30af:=diff(mR30af(t),t) = R30af, mR30af(0) = startconc:
> D_mR30ag:=diff(mR30ag(t),t) = R30ag, mR30ag(0) = startconc:
> D_mR30ah:=diff(mR30ah(t),t) = R30ah, mR30ah(0) = startconc:
> D_mR30ba:=diff(mR30ba(t),t) = R30ba, mR30ba(0) = startconc:
> D_mR30bb:=diff(mR30bb(t),t) = R30bb, mR30bb(0) = startconc:
> D_mR30bc:=diff(mR30bc(t),t) = R30bc, mR30bc(0) = startconc:
> D_mR30bd:=diff(mR30bd(t),t) = R30bd, mR30bd(0) = startconc:
> D_mR30be:=diff(mR30be(t),t) = R30be, mR30be(0) = startconc:
> D_mR30bf:=diff(mR30bf(t),t) = R30bf, mR30bf(0) = startconc:
> D_mR30bg:=diff(mR30bg(t),t) = R30bg, mR30bg(0) = startconc:
> D_mR30bh:=diff(mR30bh(t),t) = R30bh, mR30bh(0) = startconc:
> D_mR30ca:=diff(mR30ca(t),t) = R30ca, mR30ca(0) = startconc:
> D_mR30cb:=diff(mR30cb(t),t) = R30cb, mR30cb(0) = startconc:
```

```
> D_mR30cc:=diff(mR30cc(t),t) = R30cc, mR30cc(0) = startconc:
> D_mR30cd:=diff(mR30cd(t),t) = R30cd, mR30cd(0) = startconc:
> D_mR30ce:=diff(mR30ce(t),t) = R30ce, mR30ce(0) = startconc:
> D_mR30cf:=diff(mR30cf(t),t) = R30cf, mR30cf(0) = startconc:
> D_mR30cg:=diff(mR30cg(t),t) = R30cg, mR30cg(0) = startconc:
> D_mR30ch:=diff(mR30ch(t),t) = R30ch, mR30ch(0) = startconc:
> D_mR31a:=diff(mR31a(t),t) = R31a, mR31a(0) = startconc:
> D_mR32a:=diff(mR32a(t),t) = R32a, mR32a(0) = startconc:
> D_mR32b:=diff(mR32b(t),t) = R32b, mR32b(0) = startconc:
> D_mR32c:=diff(mR32c(t),t) = R32c, mR32c(0) = startconc:
> D_mR32d:=diff(mR32d(t),t) = R32d, mR32d(0) = startconc:
> D_mR32e:=diff(mR32e(t),t) = R32e, mR32e(0) = startconc:
> D_mR32f:=diff(mR32f(t),t) = R32f, mR32f(0) = startconc:
> D_mR33a:=diff(mR33a(t),t) = R33a, mR33a(0) = startconc:
> D_mR33b:=diff(mR33b(t),t) = R33b, mR33b(0) = startconc:
> D_mR33c:=diff(mR33c(t),t) = R33c, mR33c(0) = startconc:
> D_mR33d:=diff(mR33d(t),t) = R33d, mR33d(0) = startconc:
```

The differential equations are gathered into a system of differential equations, Dsys

```
> Dsys:= [D_CH3ONO, D_CH3O, D_NO, D_CH2DONO, D_CH2DO, D_CH2O,
D_HO2, D_DO2, D_CHDO, D_OH, D_NO2, D_OD, D_C6H12, D_H2O, D_RO2,
D_HDO, D_RO, D_O_atom, D_O3, D_CO, D_H2, D_HD, D_PNA, D_PNAD,
D_HOCH2O2, D_DOCH2O2, D_HOCHDO2, D_DOCHDO2, D_HCOOH, D_HCOOD,
D_DCOOH, D_DCOOD, D_CH3ONO2, D_CH2DONO2, D_D2O, D_H2O2, D_HDO2,
D_D2O2, D_HONO, D_DONO, D_CH2OHOH, D_CHDOHOH, D_CH2OHOD,
D_CHDOHOD, D_CH3OH, D_CH2OH, D_CH2DOH, D_CHDOH, D_CO2, D_HOCH2OOH,
D_DOCH2OOH, D_HOCHDOOH, D_HOCHDOOD, D_DOCH2OOD, D_HOCH2O,
D_DOCH2O, D_HOCHDO, D_DOCHDO, D_HNO3, D_DNO3, D_mR02a, D_mR02b,
D_mR02c, D_mR03a, D_mR04a, D_mR08a, D_mR08b, D_mR09a, D_mR09b,
D_mR10a, D_mR10b, D_mR11a, D_mR11b, D_mR11c, D_mR11d, D_mR12a,
D_mR12b, D_mR12c, D_mR12d, D_mR15a, D_mR15b, D_mR15c, D_mR15d,
D_mR15e, D_mR15f, D_mR16a, D_mR16b, D_mR16c, D_mR16d, D_mR16e,
D_mR16f, D_mR17a, D_mR17b, D_mR17c, D_mR18a, D_mR18b, D_mR19a,
D_mR19b, D_mR19c, D_mR20a, D_mR20b, D_mR20c, D_mR20d, D_mR20e,
D_mR20f, D_mR20g, D_mR20h, D_mR20i, D_mR20j, D_mR20k, D_mR20l,
D_mR20m, D_mR20n, D_mR20o, D_mR20p, D_mR21a, D_mR21b, D_mR21c,
D_mR22a, D_mR22b, D_mR24a, D_mR25a, D_mR25b, D_mR25c, D_mR25d,
D_mR25e, D_mR25f, D_mR28a, D_mR28b, D_mR29, D_mR30aa, D_mR30ab,
D_mR30ac, D_mR30ad, D_mR30ae, D_mR30af, D_mR30ag, D_mR30ah,
D_mR30ba, D_mR30bb, D_mR30bc, D_mR30bd, D_mR30be, D_mR30bf,
D_mR30bg, D_mR30bh,D_mR30ca, D_mR30cb, D_mR30cc, D_mR30cd,
D_mR30ce, D_mR30cf, D_mR30cg, D_mR30ch, D_mR31a, D_mR32a, D_mR32b,
D_mR32c, D_mR32d, D_mR32e, D_mR32f, D_mR33a, D_mR33b, D_mR33c,
D_mR33d]:
>
```

Solution and plotting

```
> with(plots):
```

Examples

The first step is to define the calculation procedure, p. Maxfun=0 is necessesary for long time plots, stiff = true is used for so-called stiff initial value problems (IVP), where different

magnitudes will reach steady state at very different time scales.

```
> p:= dsolve(Dsys,numeric,maxfun=0,stiff=true):
```

Next the solution is found at specific times using the procedure p.
Result after 1 second:

```
> p(1);
```

Finally, extract the concentrations of each species/reaction marker at 20 s intervals.

```
> j:=0;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
> j:=1;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
> j:=2;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 0$$

$$t, C6H12(t), CH2DO(t), CH2DOH(t)$$

1, 1, 2261924302033252, 305983027, 44451484179374

21, 21, 2261962885784088, 145893615, 44427838474640

41, 41, 2261979465300249, 122496318, 44406009863028

61, 61, 2261988062330461, 109698684, 44385174005110

81, 81, 2261993679706693, 100813991, 44365133962064

101, 101, 2261997788663464, 93957304, 44345792822875

121, 121, 2262000998771187, 88345018, 44327090136815

141, 141, 2262003616363769, 83577982, 44308981257732

161, 161, 2262005815897461, 79425200, 44291430160234

181, 181, 2262007705737800, 75740808, 44274406402386

201, 201, 2262009357453107, 72426706, 44257883519362

221, 221, 2262010820731693, 69413620, 44241838042623

241, 241, 2262012131345547, 66650750, 44226248854936

261, 261, 2262013315859383, 64099671, 44211096741079

281, 281, 2262014394542761, 61730559, 44196364061873

301, 301, 2262015383213589, 59519748, 44182034510229

$$j := 1$$

$CH2DONO(t), CH2DONO2(t), CH2O(t), CH2OH(t)$

1, 1103754465501489, 93532123338, 168234236264, 3

21, 1074785382172814, 12933851521359, 1956757482858, 3

41, 1047255506289755, 28833265724039, 3185454776173, 2

61, 1020769653423665, 45166134375267, 4222446654299, 2

81, 995191117159882, 61513004800625, 5138528734783, 2

101, 970436595294673, 77713580265725, 5965665557232, 2

121, 946445898503886, 93690583570436, 6722335687947, 2

141, 923171761626396, 109402439897230, 7420698875554, 2

161, 900575098229859, 124825749151100, 8069420714784, 2

181, 878622426716879, 139947426313867, 8675018633512, 2

201, 857284344346478, 154760680490524, 9242588535868, 2

221, 836534558418005, 169262759753392, 9776233050838, 2

241, 816349235158197, 183453598619288, 10279331223821, 2

261, 796706541969554, 197334964458282, 10754717221704, 2

281, 777586313460270, 210909896653667, 11204803701623, 2

301, 758969800012376, 224182325872888, 11631669933042, 2

$$j := 2$$

$CH2OHOD(t), CH2OHOH(t), CH3O(t), CH3OH(t)$

1, 73629920, 1274152270, 38561, 7113273210

21, 2558249456, 78402045800, 20613, 7107278196

41, 5669245521, 184127999569, 17584, 7101740258

61, 9161371737, 302474321256, 15872, 7096455627

81, 12931655661, 428230557933, 14661, 7091374719

101, 16914558734, 558537134682, 13712, 7086472926

121, 21063015669, 691570571504, 12928, 7081734797

141, 25341104817, 826082171138, 12256, 7077148868

161, 29720372727, 961179020273, 11667, 7072705859

181, 34177713336, 1096203807603, 11142, 7068397913

201, 38694030563, 1230662986063, 10666, 7064218190

221, 43253339932, 1364181102943, 10232, 7060160620

241, 47842133160, 1496470248198, 9833, 7056219741

261, 52448911787, 1627308843242, 9463, 7052390578

281, 57063834442, 1756526458415, 9119, 7048668568

301, 61678443210, 1883992659680, 8796, 7045049492

```
> j:=3;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 3$$

$$CH3ONO(t), CH3ONO2(t), CHDO(t), CHDOH(t)$$

1, 176626568923, 11650949, 1281458441139, 47

21, 171919384967, 1785919789, 14979701629258, 41

41, 167447665057, 4052793975, 24440778350661, 39

61, 163146863756, 6407124133, 32455361375546, 37

81, 158994746473, 8778199343, 39558741593042, 36

101, 154977779110, 11137895818, 45992046215840, 35

121, 151086171135, 13472125546, 51894379530673, 34

141, 147312215170, 15772972402, 57357126594549, 33

161, 143649520772, 18035723479, 62445327909177, 32

181, 140092601071, 20257516531, 67207851219393, 31

201, 136636628078, 22436638541, 71682876540861, 30

221, 133277277315, 24572127508, 75901125360154, 29

241, 130010623318, 26663530871, 79887892112226, 28

261, 126833066093, 28710751350, 83664388901002, 27

281, 123741277396, 30713944539, 87248672872260, 27

301, 120732160225, 32673448613, 90656307964011, 26

```
> j:=4;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 4$$

$$CHDOHOD(t), CHDOHOH(t), CO(t), CO2(t)$$

1, 560278459, 4289054147, 301871281, 1094

21, 19549613819, 249128764203, 75241179607, 5882307

41, 43394293479, 583231260259, 233362241349, 34476106

61, 70213100561, 958240668141, 451781027089, 96743508

81, 99216364443, 1358129078837, 718898237635, 199829262

101, 129900943380, 1773981096316, 1026652870893,
    348568148

121, 161904883614, 2200037149559, 1368847260677,
    546147924

141, 194951342825, 2632299487518, 1740494189649,
    794534464

161, 228820514412, 3067868438465, 2137466835108,
    1094764184

181, 263333444503, 3504576921309, 2556282672636,
    1447153595

201, 298834834460, 3940771103013, 2993960426728,
    1851455894

221, 333721194751, 4375170341645, 3447920324797,
    2306981678

241, 369366004123, 4806773040943, 3915911363513,
      2812693902

261, 405186156961, 5234790953425, 4395956454134,
      3367283678

281, 441104276122, 5658601903038, 4886309910142,
      3969231471

301, 477053627794, 6077714857374, 5385423739294,
      4616856905

```
> j:=5;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 5$$

$$D2O(t), D2O2(t), DCOOD(t), DCOOH(t)$$

1, 83191165, 10906750, 560278460, 4289054156

21, 1585459647, 17183551, 19549613827, 249128764284

41, 3316259179, 18112558, 43394293489, 583231260385

61, 5315971788, 18667663, 70213100574, 958240668304

81, 7555912414, 19071008, 99216364458, 1358129079033

101, 10008484364, 19390077, 129900943397, 1773981096542

121, 12649022109, 19654687, 161904883634, 2200037149811

141, 15455666071, 19880781, 194951342847, 2632299487794

161, 18408961091, 20077959, 228820514435, 3067868438764

181, 21491481227, 20252491, 263333444528, 3504576921628

201, 24687531634, 20408724, 298341834486, 3940771103351

221, 27982915925, 20549807, 333721194779, 4375170342002

241, 31364750751, 20678111, 369366004152, 4806773041317

261, 34821314819, 20795468, 405186156991, 5234790953815

281, 38341923447, 20903329, 441104276154, 5658601903443

301, 41916822478, 21002867, 477053627827, 6077714857793

```
> j:=6;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 6$$

$$DNO3(t), DO2(t), DOCH2O(t), DOCH2O2(t)$$

1, 133570904, 13838560691, 0, 0

21, 19156877614, 1828974810, 1, 0

41, 45991402012, 1302614261, 1, 0

61, 76132063342, 1077490063, 1, 0

81, 108445873904, 944040950, 1, 0

101, 142334372819, 852241760, 1, 0

121, 177406091405, 783448515, 2, 0

141, 213377398077, 728959635, 2, 0

161, 250030253161, 684105195, 2, 0

181, 287190512586, 646125805, 2, 0

201, 324715418053, 613273270, 2, 0

221, 362485764630, 584377669, 2, 0

241, 400400671184, 558622419, 2, 0

261, 438373912405, 535417325, 3, 0

281, 476331242580, 514322934, 3, 0

301, 514208378432, 495003690, 3, 0

```
> j:=7;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 7$$

$$DOCH2OOD(t), DOCH2OOH(t), DOCHDO(t), DOCHDO2(t)$$

1, 0, 0, 1, 2

21, 0, 1, 5, 2

41, 0, 2, 7, 2

61, 0, 3, 8, 2

81, 0, 3, 10, 2

101, 0, 3, 11, 2

121, 0, 4, 13, 2

141, 0, 4, 14, 2

161, 0, 5, 15, 2

181, 0, 5, 16, 2

201, 0, 5, 17, 2

221, 0, 5, 18, 3

241, 0, 6, 19, 3

261, 0, 6, 20, 3

281, 0, 6, 21, 3

301, 1, 6, 21, 3

```
> j:=8;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 8$$

$$DONO(t), H2(t), H2O(t), H2O2(t)$$

1, 644149, 4698551, 609771698617, 50973299482

21, 89082255, 1262988458, 14344935699541, 118641330020

41, 198606976, 4062769682, 27204071277149, 134135832489

61, 311135687, 8076018109, 39531601709379, 143387715194

81, 423778591, 13140008413, 51421632323505, 149928527252

101, 535430508, 19143221890, 62921775827631, 154929884479

121, 645557987, 26000348538, 74062183558392, 158933573917

141, 753873498, 33642253543, 84865544287747, 162237351508

161, 860214731, 42010882664, 95350481425345, 165023329293

181, 964490484, 51056295413, 105532948541651,
        167411329673

201, 1066652967, 60734774125, 115426966448352,
        169484507910

221, 1166682270, 71007538734, 125045079731725,
        171302968638

241, 1264577043, 81839830144, 134398661172373,
        172911574164

261, 1360348621, 93200231444, 143498126671656,
        174344691959

281, 1454017152, 105060149913, 152353092934781,
        175629220622

301, 1545608972, 117393411866, 160972496528969,
        176786595685

```
> j:=9;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 9$$

$$HCOOD(t), HCOOH(t), HD(t), HDO(t)$$

1, 707538300, 6837358689, 19648213, 80802114023

21, 24666112733, 405932855827, 5305740608, 1179114232728

41, 54732784522, 951487259436, 17097333232, 2106925911329

61, 88535844037, 1563189310704, 34032453110,
        3000373109815

81, 125079675767, 2214590194764, 55436918865,
        3876452499346

101, 163730060850, 2891055365752, 80849067395,
    4740364697628

121, 204030914954, 3583178292646, 109915757817,
    5593933544548

141, 245633552462, 4284463829881, 142350697569,
    6437761790701

161, 288261259869, 4990226479104, 177913318984,
    7271952343188

181, 331688871179, 5696984536615, 216396497361,
    8096393117685

201, 375729895590, 6402097075245, 257618734071,
    8910884454115

221, 420227874618, 7103532547643, 301418850522,
    9715200621702

241, 465050270446, 7799713537457, 347652208546,
    10509120350722

261, 510083980538, 8489408640030, 396187914630,
    11292441882186

281, 555231945011, 9171654819993, 446906688638,
    12064989905835

301, 600410514217, 9845700176864, 499699198362,
    12826618116715

```
> j:=10;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 10$$

$$HDO2(t), HNO3(t), HO2(t), HOCH2O(t)$$

1, 3473724691, 460941898, 118404461708, 2

21, 6481087915, 111159355313, 25354322196, 16

41, 7040748290, 279647011929, 18298300173, 26

61, 7375080413, 469003298318, 14975538144, 33

81, 7614723670, 669555832265, 12908533095, 40

101, 7801116738, 876560622342, 11447936250, 46

121, 7952997912, 1087226922280, 10337873621, 51

141, 8080537768, 1299717494970, 9453633468, 56

161, 8189917677, 1512752161799, 8725766952, 60

181, 8285196442, 1725401689159, 8111904958, 65

201, 8369193680, 1936972036634, 7584461159, 68

221, 8443954061, 2146934369171, 7124526583, 72

241, 8511011266, 2354880155513, 6718630222, 75

261, 8571547468, 2560491019604, 6356861786, 79

281, 8626494531, 2763517730009, 6031727712, 82

301, 8676600883, 2963765092534, 5737430213, 84

```
> j:=11;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 11$$

$$HOCH2O2(t),\ HOCH2OOH(t),\ HOCHDO(t),\ HOCHDO2(t)$$

1, 5, 4, 6, 16

21, 8, 41, 53, 26

41, 9, 64, 82, 28

61, 9, 83, 106, 29

81, 9, 100, 127, 30

101, 9, 114, 146, 30

121, 10, 128, 163, 31

141, 10, 140, 179, 31

161, 10, 151, 193, 31

181, 9, 161, 206, 31

201, 9, 171, 219, 31

221, 9, 180, 231, 31

241, 9, 188, 242, 30

261, 9, 196, 252, 30

281, 9, 204, 262, 30

301, 9, 211, 271, 30

```
> j:=12;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 12$$

$$HOCHDOOD(t), HOCHDOOH(t), HONO(t), NO(t)$$

1, 2, 15, 10308317, 748247829118

21, 11, 131, 1425611309, 3251763249358

41, 17, 205, 3178381646, 4310984772655

61, 21, 265, 4979230387, 5080138672938

81, 25, 318, 6781909054, 5703189570048

101, 28, 365, 8568730132, 6233494906760

121, 32, 407, 10331156090, 6697991645688

141, 34, 446, 12064585081, 7112549426221

161, 37, 482, 13766419411, 7487398404099

181, 40, 516, 15435199352, 7829567307690

201, 42, 547, 17070159970, 8144129274700

221, 45, 576, 18670982535, 8434888131321

241, 47, 604, 20237645401, 8704786721781

261, 49, 630, 21770329874, 8956160500327

281, 51, 654, 23269358342, 9190902031233

301, 53, 677, 24735152261, 9410572443005

```
> j:=13;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 13$$

$$NO2(t), O3(t), OD(t), OH(t)$$

1, 536439215853, 687703109, 5419270, 46450900

21, 4348790891062, 118477693498, 3023230, 42513129

41, 5475948533292, 177941915801, 2823407, 40375020

61, 6172295589330, 185405065934, 2730999, 38722294

81, 6681638064450, 180386714557, 2669708, 37297873

101, 7085279625882, 174566581265, 2620489, 36007905

121, 7420215430546, 169667660982, 2576685, 34814124

141, 7706451865626, 165609518979, 2535527, 33697111

161, 7956120911298, 162181543965, 2495722, 32644679

181, 8177180066961, 159232118693, 2456627, 31648161

201, 8375150369160, 156658193636, 2417920, 30701056

221, 8554031728718, 154387196712, 2379443, 29798221

241, 8716821297288, 152366051254, 2341127, 28935508

261, 8865827659063, 150554715299, 2302957, 28109490

281, 9002870821075, 148922192568, 2264941, 27317263

301, 9129414035039, 147443965040, 2227102, 26556320

```
> j:=14;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 14$$

$$O\_atom(t), PNA(t), PNAD(t), RO(t)$$

1, 36927, 154710390524, 20029801582, 4036928862

21, 299370, 9135350431629, 723994056647, 10483932727

41, 376963, 17768173869427, 1340273512116, 10355969107

61, 424899, 25671089133757, 1905367661299, 10089720106

81, 459962, 33005503472160, 2437235174096, 9807467993

101, 487749, 39877380629110, 2944223036944, 9527397026

121, 510806, 46358780665491, 3431030758144, 9254741351

141, 530510, 52501841616715, 3900625635915, 8991330910

161, 547697, 58346169445637, 4355038180460, 8737619247

181, 562915, 63922981188114, 4795745021454, 8493462018

201, 576543, 69257594111162, 5223872506053, 8258497361

221, 588857, 74371009984874, 5640313420583, 8032268780

241, 600064, 79280971641117, 6045798007152, 7814312541

261, 610321, 84002695364497, 6440939276144, 7604182773

281, 619755, 88549395055303, 6826263071741, 7401454507

301, 628467, 92932667774861, 7202228691428, 7205726987

```
> j:=15;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 15$$

$$RO2(t),\ mR02a(t),\ mR02b(t),\ mR02c(t)$$

1, 109584037860, 236912389, 168621781606, 1280345188601

21, 64553283160, 3119229545, 2019483348353, 15333937074456

41, 48101730618, 5277841483, 3349053618122, 25429364139673

61, 39770949407, 7180651773, 4507970352834, 34229018912315

81, 34435825284, 8920121656, 5560711664847, 42222483699859

101, 30606939479, 10537650488, 6535497025781, 49624028950460

121, 27669487433, 12056944946, 7448238896601, 56554477980300

141, 25315305291, 13493496990, 8309211199028, 63091840677070

161, 23369483262, 14858301916, 9125632738158, 69290929427891

181, 21723800150, 16159616731, 9902877572916, 75192549462216

201, 20307049500, 17403902087, 10645118424414, 80828384251470

221, 19069999496, 18596373214, 11355700532286, 86223834200205

241, 17977341881, 19741344190, 12037373926481, 91399780285848

261, 17002957813, 20842454355, 12692445392067, 96373737927420

281, 16127002701, 21902823482, 13322882126603, 101160644056002

301, 15334059392, 22925161839, 13930384944508,
    105773412955488

```
> j:=16;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 16$$

$$mR03a(t), mR04a(t), mR08a(t), mR08b(t)$$

1, 610911995041, 599782801110, 4698552, 19648214

21, 14476121265933, 14062416657612, 1262991466,
    5305746500

41, 27528392109314, 26605783070536, 4062787870,
    17097368926

61, 40073814547465, 38585398416720, 8076070321,
    34032555699

81, 52195985271866, 50102331787025, 13140118337,
    55437135040

101, 63937224535477, 61209318516003, 19143416906,
    80849451197

121, 75324432101547, 71940540244988, 26000658873,
    109916368969

141, 86378096024523, 82321937876893, 33642711611,
    142351600184

161, 97115259587352, 92374811660150, 42011522542,
    177914580527

181, 107550695173258, 102117354730922, 51057152406,
    216398187800

201, 117697515074746, 111565485154595, 60735884411,
    257620925169

221, 127567550630707, 120733369843142, 71008939058,
    301421615237

241, 137171606307271, 129633778688692, 81841557568,
    347655620530

261, 146519640358279, 138278337268875, 93202323126,
    396192047793

281, 155620898298108, 146677713966227, 105062642921,
    446911616780

301, 164484014310334, 154841762460557, 117396343024,
    499704994858

```
> j:=17;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 17$$

$$mR09a(t), mR09b(t), mR10a(t), mR10b(t)$$

1, 1566184, 10836288, 154710390524, 20029801582

21, 420997155, 2926199584, 9135350431629, 723994056647

41, 1354262623, 9429458011, 17768173869427, 1340273512116

61, 2692023440, 18769470109, 25671089133757,
    1905367661299

81, 4380039446, 30574419925, 33005503472160,
    2437235174096

101, 6381138969, 44589697317, 39877380629110,
    2944223036944

121, 8666886291, 60620542873, 46358780665491,
    3431030758144

141, 11214237204, 78509064327, 52501841616715,
    3900625635915

161, 14003840847, 98122586815, 58346169445637,
    4355038180460

181, 17019050802, 119346879307, 63922981188114,
    4795745021454

201, 20245294804, 142081843548, 69257594111162,
    5223872506053

221, 23669646353, 166238587763, 74371009984874,
    5640313420583

241, 27280519189, 191737342191, 79280971641117,
    6045798007152

261, 31067441042, 218505917222, 84002695364497,
    6440939276144

281, 35020880974, 246478527990, 88549395055303,
    6826263071741

301, 39132114341, 275594875894, 92932667774861,
    7202228691428

```
> j:=18;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 18$$

$$mR11a(t), mR11b(t), mR11c(t), mR11d(t)$$

1, 1127258759, 147259875, 8578110254, 1120557174

21, 65191966585, 5116499651, 498257599205, 39099233282

41, 152371951034, 11338492533, 1166462672149, 86788598371

61, 250033450163, 18322745763, 1916481573553,
    140426218660

81, 354000799468, 25863314445, 2716258483365,
    198432752835

101, 461957435656, 33829121454, 3547962608469,
    259801917361

121, 572411264103, 42126036212, 4400074806178,
    323809804682

141, 684330083375, 50682215417, 5264599573958,
    389902730127

161, 796967999961, 59440752164, 6135737568044,
    457641080469

181, 909769872415, 68355434325, 7009154626025,
    526666947945

201, 1022313990747, 77388069734, 7881543081651,
    596683735261

221, 1134275494999, 86506689436, 8750341650928,
    667442463336

241, 1245401802425, 95684276867, 9613547141220,
    738732089653

261, 1355549473484, 104897835104, 10469583057483,
    810372402970

281, 1464401892618, 114127681404, 11317205047542,
    882208648991

301, 1572000176287, 123356899933, 12155431046528,
    954107360080

```
> j:=19;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 19$$

$$mR12a(t), mR12b(t), mR12c(t), mR12d(t)$$

$$1, 0, 0, 0, 0$$

$$21, 1, 0, 2, 0$$

$$41, 1, 0, 3, 0$$

$$61, 1, 0, 5, 0$$

$$81, 2, 0, 6, 0$$

$$101, 2, 0, 7, 1$$

$$121, 2, 0, 8, 1$$

$$141, 3, 0, 8, 1$$

$$161, 3, 0, 9, 1$$

$$181, 3, 0, 10, 1$$

$$201, 3, 0, 11, 1$$

$$221, 3, 0, 11, 1$$

$$241, 4, 0, 12, 1$$

$$261, 4, 0, 12, 1$$

$$281, 4, 0, 13, 1$$

$$301, 4, 0, 13, 1$$

```
> j:=20;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 20$$

$$mR15a(t),\ mR15b(t),\ mR15c(t),\ mR15d(t)$$

1, 2098317, 8741645543, 546352846, 71832765

21, 48545903, 202284473691, 12642779606, 1022907601

41, 90678858, 377921018293, 23620063643, 1793927123

61, 129877433, 541391520206, 33836970013, 2510771879

81, 166598265, 694590816547, 43411926034, 3190857150

101, 201113850, 838647651795, 52415478237, 3840592378

121, 233621656, 974378955343, 60898684709, 4463149909

141, 264282058, 1102447719391, 68902982462, 5060464624

161, 293232220, 1223420799759, 76463799985, 5633913335

181, 320592497, 1337795483536, 83612217721, 6184589752

201, 346470143, 1446014905027, 90375931564, 6713431201

221, 370961782, 1548478273225, 96779892077, 7221282227

241, 394155155, 1645548135127, 102846758446, 7708928174

261, 416130436, 1737755798646, 108597237415, 8177113522

281, 436961242, 1824805525072, 114050345317, 8626552098

301, 456715439, 1907577859525, 119223616220, 9057932789

```
> j:=21;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 21$$

$$mR15e(t), mR15f(t), mR16a(t), mR16b(t)$$

1, 1149324244, 275880, 33814241, 178735579

21, 16366521609, 3927838, 8712647223, 46258742448

41, 28702833967, 6887163, 26913568019, 143141240792

61, 40172350071, 9637436, 51856762126, 276170922002

81, 51053714408, 12245624, 82125851835, 437872784988

101, 61449478047, 14736416, 116737738490, 623049622343

121, 71410398541, 17122067, 154939300509, 827711949863

141, 80967433984, 19410075, 196127869241, 1048660467608

161, 90142613353, 21605793, 239808078397, 1283259727751

181, 98953436032, 23713484, 285564967638, 1529297099055

201, 107414899217, 25736805, 333046074048, 1784888885841

221, 115540515632, 27679056, 381948900952, 2048414651828

241, 123342850778, 29543305, 432011759057, 2318469221100

261, 130833816348, 31332460, 483006850345, 2593826429434

281, 138024833565, 33049310, 534734905813, 2873411012924

301, 144926924618, 34696541, 587020934558, 3156276314090

```
> j:=22;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 22$$

$$mR16c(t), mR16d(t), mR16e(t), mR16f(t)$$

1, 22341947, 2875469, 23003749, 4352151

21, 5782342806, 435656477, 3485251817, 656486441

41, 17892655098, 1285703092, 10285624734, 1934048295

61, 34521365248, 2452676308, 19621410469, 3684514885

81, 54734098120, 3888731047, 31109848376, 5835039801

101, 77881202788, 5559531809, 44476254473, 8333384773

121, 103463993726, 7437361588, 59498892705, 11137453233

141, 131082558442, 9498730380, 75989843044, 14211642109

161, 160407465958, 11723195661, 93785565293, 17525035547

181, 191162137369, 14092668153, 112741345232, 21050338526

201, 223111110715, 16590964114, 132727712923, 24763187115

221, 256051831461, 19203495934, 153627967483, 28641670481

241, 289808652618, 21917045094, 175336360764, 32665979388

261, 324228303657, 24719587730, 197756701854, 36818135704

281, 359176376591, 27600155666, 220801245346, 41081776714

301, 394534539235, 30548722458, 244389779677, 45441978182

```
> j:=23;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 23$$

$$mR17a(t),\ mR17b(t),\ mR17c(t),\ mR18a(t)$$

1, 50973451453, 3473735212, 10906783, 151971

21, 118652387643, 6481726314, 17185318, 11057623

41, 134160813649, 7042129978, 18116262, 24981160

61, 143427916233, 7377252125, 18673381, 40201039

81, 149984796301, 7617716239, 19078792, 56269049

101, 155002846367, 7804953241, 19399967, 72961888

121, 159023717894, 7957696739, 19666713, 90143976

141, 162345075376, 8086114139, 19894971, 107723867

161, 165148964964, 8196384513, 20094336, 125635671

181, 167555159372, 8292564909, 20271075, 143829699

201, 169646775116, 8377473569, 20429533, 162267205

221, 171483885832, 8453154042, 20572857, 180917194

241, 173111328520, 8521139086, 20703417, 199754356

261, 174563449645, 8582610101, 20823043, 218757686

281, 175867130130, 8638498288, 20933186, 237909508

301, 177043790461, 8689551507, 21035018, 257194776

```
> j:=24;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 24$$

$$mR18b(t), mR19a(t), mR19b(t), mR19c(t)$$

1, 10521, 1926, 10306391, 644149

21, 638399, 295224, 1425316085, 89082255

41, 1381688, 670034, 3177711613, 198606976

61, 2171711, 1059390, 4978170997, 311135687

81, 2992569, 1451601, 6780457453, 423778591

101, 3836503, 1842013, 8566888119, 535430508

121, 4698827, 2228292, 10328927798, 645557987

141, 5576372, 2609123, 12061975958, 753873498

161, 6466835, 2983722, 13763435689, 860214731

181, 7368468, 3351610, 15431847742, 964490484

201, 8279889, 3712499, 17066447470, 1066652967

221, 9199981, 4066226, 18666916308, 1166682270

241, 10127821, 4412712, 20233232689, 1264577043

261, 11062633, 4751935, 21765577939, 1360348621

281, 12003757, 5083918, 23264274424, 1454017152

301, 12950624, 5408714, 24729743548, 1545608972

```
> j:=25;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 25$$

$$mR20a(t), \, mR20b(t), \, mR20c(t), \, mR20d(t)$$

1, 262011012, 881896181, 15128156, 115116920

21, 17585295639, 55869035074, 572520914, 4375194173

41, 41532078692, 131542781090, 1277157461, 9775982326

61, 68277840663, 216293225490, 2066360392, 15836894712

81, 96598281639, 306348428238, 2915427547, 22368420510

101, 125832204523, 399643580347, 3808975227, 29252374586

121, 155564514543, 494864880369, 4736128844, 36405047747

141, 185515575670, 591114590490, 5688705052, 43763299926

161, 215488889590, 687752170319, 6660307661, 51277652703

181, 245342508512, 784307162111, 7645808766, 58908328213

201, 274972034357, 880427162964, 8641023239, 66622765503

221, 304299871112, 975844779283, 9642491199, 74393961349

241, 333268078718, 1070355541492, 10647324968,
    82199303020

261, 361833443687, 1163802586109, 11653097350,
    90019716096

281, 389963974660, 1256065702829, 12657757589,
    97839023336

301, 417636346333, 1347053296840, 13659566561,
    105643449946

```
> j:=26;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 26$$

$$mR20e(t), mR20f(t), mR20g(t), mR20h(t)$$

1, 881896181, 2968536340, 50946766, 387674861

21, 55869035074, 177517778805, 1821593124, 13920357200

41, 131542781090, 416652923281, 4048297467, 30987258421

61, 216293225490, 685205546997, 6549087396, 50192808257

81, 306348428238, 971569319970, 9249021970, 70962308659

101, 399643580347, 1269305438246, 12100646222,
    92931431502

121, 494864880369, 1574263415380, 15069984432,
    115838869378

141, 591114590490, 1883568495133, 18131167487,
    139485234408

161, 687752170319, 2195139978172, 21263747139,
    163712542836

181, 784307162111, 2507426198660, 24451149172,
    188392411366

201, 880427162964, 2819245609915, 27679699489,
213418630645

221, 975844779283, 3129685405179, 30937970825,
238702186358

241, 1070355541492, 3438033435041, 34216321289,
264167743121

261, 1163802586109, 3743730744124, 37506556077,
289751067116

281, 1256065702829, 4046337449444, 40801671911,
315397078854

301, 1347053296840, 4345507557653, 44095659020,
341058343861

```
> j:=27;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 27$$

$$mR20i(t), mR20j(t), mR20k(t), mR20l(t)$$

1, 15128156, 50946766, 877561, 6677437

21, 572520914, 1821593124, 18996282, 145139136

41, 1277157461, 4048297467, 39730607, 304059987

61, 2066360392, 6549087396, 63018386, 482905563

81, 2915427547, 9249021970, 88474748, 678731397

101, 3808975227, 12100646222, 115787331, 889149954

121, 4736128844, 15069984432, 144700068, 1112202324

141, 5688705052, 18131167487, 174997157, 1346235121

161, 6660307661, 21263747139, 206493139, 1589824788

181, 7645808766, 24451149172, 239026482, 1841728916

201, 8641023239, 27679699489, 272455146, 2100852689

221, 9642491199, 30937970825, 306653362, 2366224546

241, 10647324968, 34216321289, 341509182, 2636977720

261, 11653097350, 37506556077, 376922558, 2912335803

281, 12657757589, 40801671911, 412803802, 3191601140

301, 13659566561, 44095659020, 449072321, 3474145309

```
> j:=28;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 28$$

$$mR20m(t), mR20n(t), mR20o(t), mR20p(t)$$

1, 115116920, 387674861, 6677437, 50809241

21, 4375194173, 13920357200, 145139136, 1108923311

41, 9775982326, 30987258421, 304059987, 2326992745

61, 15836894712, 50192808257, 482905563, 3700492029

81, 22368420510, 70962308659, 678731397, 5206903877

101, 29252374586, 92931431502, 889149954, 6827987339

121, 36405047747, 115838869378, 1112202324, 8548764165

141, 43763299926, 139485234408, 1346235121, 10356573371

161, 51277652703, 163712542836, 1589824788, 12240494085

181, 58908328213, 188392411366, 1841728916, 14190976008

201, 66622765503, 213418630645, 2100852689, 16199585623

221, 74393961349, 238702186358, 2366224546, 18258822498

241, 82199303020, 264167743121, 2636977720, 20361980261

261, 90019716096, 289751067116, 2912335803, 22503037946

281, 97839023336, 315397078854, 3191601140, 24676572792

301, 105563449946, 341058343861, 3474145309, 26877688678

```
> j:=29;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 29$$

$$mR21a(t), mR21b(t), mR21c(t), mR22a(t)$$

1, 247740, 64505732, 1032091706, 73266902

21, 5806046, 1511996266, 24191940252, 1640478728

41, 10980550, 2859940475, 45759047600, 3088634315

61, 15918701, 4146677533, 66346840522, 4470938477

81, 20662648, 5383144417, 86130310676, 5800312140

101, 25234505, 6575067464, 105201079422, 7083154244

121, 29648679, 7726170366, 123618725844, 8323474247

141, 33916141, 8839285069, 141428561099, 9524243028

161, 38045918, 9916739973, 158667839567, 10687862938

181, 42045731, 10960525584, 175368409333, 11816366712

201, 45922341, 11972384538, 191558152596, 12911522960

221, 49681769, 12953868368, 207261893883, 13974900789

241, 53329446, 13906375922, 222502014747, 15007912421

261, 56870316, 14831180811, 237298892966, 16011842974

281, 60308914, 15729451761, 251671228165, 16987872108

301, 63649430, 16602268132, 265636290095, 17937090266

```
> j:=30;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 30$$

$$mR22b(t), mR24a(t), mR25a(t), mR25b(t)$$

1, 1167785449, 1065, 1, 1

21, 26147254445, 5789964, 2783, 4359

41, 49229136831, 33954312, 16871, 26467

61, 71261449335, 95285781, 48447, 76088

81, 92450133399, 196803087, 101958, 160281

101, 112897178373, 343243426, 180766, 284413

121, 132666488363, 537719233, 287435, 452598

141, 151805414002, 782139187, 423915, 667986

161, 170352244410, 1077497554, 591668, 932959

181, 188339377653, 1424081341, 791754, 1249269

201, 205795002061, 1821624944, 1024907, 1618147

221, 222744126204, 2269429243, 1291584, 2040384

241, 239209258247, 2766455192, 1592008, 2516407

261, 255210880494, 3311398448, 1926208, 3046323

281, 270767794477, 3902749556, 2294046, 3629978

301, 285897379782, 4538842885, 2695241, 4266988

```
> j:=31;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 31$$

$$mR25c(t), mR25d(t), mR25e(t), mR25f(t)$$

1, 0, 0, 0, 0

21, 1168, 225, 288, 77

41, 7093, 1317, 1683, 451

61, 20392, 3765, 4818, 1291

81, 42955, 7965, 10204, 2735

101, 76223, 14250, 18270, 4896

121, 121296, 22900, 29384, 7875

141, 179020, 34153, 43855, 11753

161, 250033, 48210, 61948, 16602

181, 334804, 65239, 83885, 22481

201, 433663, 85378, 109848, 29439

221, 546823, 108741, 139991, 37518

241, 674397, 135416, 174433, 46748

261, 816415, 165473, 213269, 57156

281, 972834, 198962, 256569, 68760

301, 1143553, 235917, 304381, 81574

```
> j:=32;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 32$$

$$mR28a(t), mR28b(t), mR29(t), mR30aa(t)$$

1, 401213388950, 52788951251, 110895363672, 4

21, 3105280707095, 281739533783, 11733627778583, 38

41, 3932919725149, 340856064895, 24286580303408, 59

61, 4437252017450, 376908141379, 36574183188898, 77

81, 4796625857921, 402960833078, 48528805473237, 93

101, 5072558290980, 423313031383, 60144751501236, 106

121, 5294016163818, 439942747607, 71428317672158, 119

141, 5477089456761, 453934883780, 82389717945139, 130

161, 5631687484268, 465953443873, 93040421363786, 140

181, 5764361389591, 476436593674, 103392031818425, 150

201, 5879673085591, 485689833042, 113455825216063, 159

221, 5980928093216, 493935301553, 123242575839434, 167

241, 6070598144358, 501339966296, 132762504587054, 175

261, 6150579266862, 508032727450, 142025281342476, 182

281, 6222356868742, 514115311227, 151040050089253, 189

301, 6287115483103, 519669490137, 159815462226544, 195

```
> j:=33;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 33$$

$$mR30ab(t), mR30ac(t), mR30ad(t), mR30ae(t)$$

1, 1, 0, 0, 13

21, 3, 1, 0, 121

41, 5, 2, 0, 189

61, 6, 3, 0, 246

81, 7, 3, 0, 295

101, 8, 3, 0, 338

121, 9, 4, 0, 378

141, 10, 4, 0, 414

161, 11, 5, 0, 448

181, 12, 5, 0, 479

201, 12, 5, 0, 508

221, 13, 5, 0, 535

241, 14, 6, 0, 560

261, 14, 6, 0, 584

281, 15, 6, 0, 606

301, 15, 6, 1, 628

```
> j:=34;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 34$$

$$mR30af(t), mR30ag(t), mR30ah(t), mR30ba(t)$$

1, 2, 2, 0, 2

21, 11, 11, 1, 23

41, 15, 15, 1, 36

61, 19, 19, 2, 46

81, 23, 23, 2, 56

101, 26, 26, 2, 64

121, 29, 29, 2, 71

141, 32, 32, 3, 78

161, 35, 35, 3, 84

181, 37, 37, 3, 90

201, 39, 39, 3, 95

221, 42, 42, 3, 100

241, 44, 44, 3, 105

261, 46, 46, 4, 109

281, 48, 48, 4, 113

301, 49, 49, 4, 117

```
> j:=35;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 35$$

$$mR30bb(t), mR30bc(t), mR30bd(t), mR30be(t)$$

1, 0, 0, 0, 8

21, 2, 1, 0, 73

41, 3, 1, 0, 114

61, 4, 2, 0, 147

81, 4, 2, 0, 177

101, 5, 2, 0, 203

121, 5, 2, 0, 227

141, 6, 3, 0, 249

161, 6, 3, 0, 269

181, 7, 3, 0, 287

201, 7, 3, 0, 305

221, 8, 3, 0, 321

241, 8, 3, 0, 336

261, 9, 4, 0, 350

281, 9, 4, 0, 364

301, 9, 4, 0, 377

```
> j:=36;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 36$$

$$mR30bf(t), mR30bg(t), mR30bh(t), mR30ca(t)$$

1, 1, 1, 0, 2

21, 6, 6, 1, 15

41, 9, 9, 1, 24

61, 12, 12, 1, 31

81, 14, 14, 1, 37

101, 16, 16, 1, 43

121, 18, 18, 1, 47

141, 19, 19, 2, 52

161, 21, 21, 2, 56

181, 22, 22, 2, 60

201, 24, 24, 2, 64

221, 25, 25, 2, 67

241, 26, 26, 2, 70

261, 27, 27, 2, 73

281, 29, 29, 2, 76

301, 30, 30, 2, 78

```
> j:=37;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 37$$

$$mR30cb(t), mR30cc(t), mR30cd(t), mR30ce(t)$$

1, 0, 0, 0, 5

21, 1, 1, 0, 48

41, 2, 1, 0, 76

61, 2, 1, 0, 98

81, 3, 1, 0, 118

101, 3, 1, 0, 135

121, 4, 2, 0, 151

141, 4, 2, 0, 166

161, 4, 2, 0, 179

181, 5, 2, 0, 192

201, 5, 2, 0, 203

221, 5, 2, 0, 214

241, 5, 2, 0, 224

261, 6, 2, 0, 234

281, 6, 2, 0, 243

301, 6, 3, 0, 251

```
> j:=38;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 38$$

$$mR30cf(t), mR30cg(t), mR30ch(t), mR31a(t)$$

1, 1, 1, 0, 460941898

21, 4, 4, 0, 111159355313

41, 6, 6, 1, 279647011929

61, 8, 8, 1, 469013298318

81, 9, 9, 1, 669555832265

101, 10, 10, 1, 876560622342

121, 12, 12, 1, 1087226922280

141, 13, 13, 1, 1299717494970

161, 14, 14, 1, 1512752161799

181, 15, 15, 1, 1725401689159

201, 16, 16, 1, 1936972036634

221, 17, 17, 1, 2146934369171

241, 17, 17, 1, 2354880155513

261, 18, 18, 1, 2560491019604

281, 19, 19, 2, 2763517730009

301, 20, 20, 2, 2963765092534

```
> j:=39;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 39$$

$$mR32a(t), mR32b(t), mR32c(t), mR32d(t)$$

1, 49, 16520, 264318, 6

21, 207799, 63541958, 1016671323, 15322

41, 927058, 278168872, 4450701946, 65789

61, 2164561, 643072648, 10289162367, 152645

81, 3893853, 1149334699, 18389355181, 275524

101, 6082097, 1786770229, 28588323663, 433495

121, 8695116, 2545104753, 40721676043, 625314

141, 11699366, 3414425231, 54630803701, 849560

161, 15062724, 4385340866, 70165453856, 1104707

181, 18754762, 5449026047, 87184416753, 1389173

201, 22746827, 6597218341, 105555493455, 1701353

221, 27012027, 7822198794, 125155180701, 2039639

241, 31525175, 9116764687, 145868234989, 2402442

261, 36262711, 10474199682, 167587194905, 2788196

281, 41202620, 11888243705, 190211899272, 3195375

301, 46324340, 13353063636, 213649018179, 3622492

```
> j:=40;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]),lhs(p(1)[4*
j+4]);
for i from 1 by 20 while i < 302 do

i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2])),round(rhs(p(
i)[4*j+3])),round(rhs(p(i)[4*j+4]));
end do;
```

$$j := 40$$

$$mR32e(t), mR32f(t), mR33a(t), mR33b(t)$$

1, 2069, 33104, 568, 33

21, 4688352, 75013638, 22161, 735

41, 19747934, 315966938, 47693, 1487

61, 45359256, 725748092, 74681, 2283

81, 81332560, 1301320957, 102453, 3116

101, 127349094, 2037585506, 130670, 3978

121, 183017578, 2928281246, 159127, 4865

141, 247906005, 3966496082, 187689, 5774

161, 321560188, 5144963013, 216260, 6700

181, 403515319, 6456245100, 244775, 7641

201, 493303786, 7892860576, 273183, 8596

221, 590460724, 9447371591, 301445, 9561

241, 694528015, 11112448240, 329534, 10535

261, 805057189, 12880915021, 357427, 11517

281, 921611526, 14745784418, 385107, 12506

301, 1043767551, 16700280810, 412560, 13499

```
> j:=41;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]);
for i from 1 by 20 while i < 302 do
   i,round(rhs(p(i)[4*j+1])),round(rhs(p(i)[4*j+2]));
end do;
```

$$j := 41$$

$$mR33c(t), mR33d(t)$$

1, 1913, 251

21, 70509, 5618

41, 151190, 11377

61, 236708, 17493

81, 325020, 23898

101, 415070, 30542

121, 506207, 37388

141, 597990, 44405

161, 690110, 51568

181, 782335, 58856

201, 874491, 66252

221, 966443, 73741

241, 1058084, 81310

261, 1149331, 88946

281, 1240116, 96640

301, 1330383, 104383

>
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Comments: