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

14b. CH2DO + NO2 + M --> CH2DONO2 + M
15a. OH + CH3ONO --> CH2O + NO + H2O
15b. OH + CH2DONO --> 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.

```
>
```

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

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

1

1

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

1

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 + *hv* --> CH3O + NO

```
> j1a:=1.44e-3: R1a:=j1a*CH3ONO(t):
```

1b. CH2DONO + *hv* --> 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 --> CH2O + HO2

```
> k2a:= 1.9e-15: R2a:=k2a*CH3O(t)*O2:
```

2b. CH2DO + O2 --> CH2O + DO2

```
> k2b:= (1/7.593)*(2/3)*1.9e-15: R2b:=k2b*CH2DO(t)*O2:
```

2c. CH2DO + O2 --> 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 --> OH + NO2
```
> k3a:= 8.1e-12: R3a:=k3a*HO2(t)*NO(t):
```
3b. DO2 + NO --> OD + NO2
```
> k3b:= 8.1e-12: R3b:=k3b*DO2(t)*NO(t):
```
4a. OH + cC6H12 --> H2O + RO2
```
> k4a := 6.37e-12: R4a:=k4a*OH(t)*C6H12(t):
```
4b. OD + cC6H12 --> HDO + RO2
```
> k4b := k4a: R4b:=k4b*OD(t)*C6H12(t):
```
5. RO2 + NO --> RO + NO2
```
> k5 := 6.7e-12: R5:=k5*RO2(t)*NO(t):
```
6. NO2 + hv --> NO + O
```
> j6 := 2*j1a: R6:=j6*NO2(t):
```
7. O + O2 + M --> 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 + hv --> CO + H2
```
> j8a := 0.05*0.75*j1a: R8a:=j8a*CH2O(t):
```
8b. CHDO + hv --> CO + HD
```
> j8b := j8a/1.82: R8b:=j8b*CHDO(t):
```
9a. CH2O + hv --> CO + 2*HO2
```
> j9a := 0.05*0.25*j1a: R9a:=j9a*CH2O(t):
```
9b. CHDO + hv --> CO + HO2 + DO2
```
> j9b := j9a/1.10: R9b:=j9b*CHDO(t):
```
10a. HO2 + NO2 + M --> PNA + M
```
> k10a := 1.8e-31: R10a:=k10a*HO2(t)*NO2(t)*M:
```
10b. DO2 + NO2 + M --> PNAD + M
```
> k10b := 1.8e-31: R10b:=k10b*DO2(t)*NO2(t)*M:
```
11a. HO2 + CH2O --> HOCH2O2
```
> k11a := 8.01e-14: R11a:=k11a*HO2(t)*CH2O(t):
```
11b. DO2 + CH2O --> 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 := 2.34e-26: R13a:=k13a*CH3O(t)*NO(t)*M:
```
13b. CH2DO + NO + M --> CH2DONO + M
```
> k13b := 2.34e-26: R13b:=k13b*CH2DO(t)*NO(t)*M:
```
14a. CH3O + NO2 + M --> CH3ONO2 + M
```
> k14a := 5.46e-26: R14a:=k14a*CH3O(t)*NO2(t)*M:
```
14b. CH2DO + NO2 + M --> CH2DONO2 + M
```
> k14b := 5.46e-26: 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 := 2.3e-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 --> DCOOD + HCOOD + HO2 + DO2
```
> k20p := 5.5e-12: R20p:=k20p*DOCHDO2(t)*DOCHDO2(t)*O2(t):
```
21a. CH3OH + OH --> CH2OH + H2O
```
k21a := 8.8e-13: R21a:=k21a*CH3OH(t)*OH(t):
```

21b. CH2DOH + OH --> CH2OH + HDO
```
> k21b := (1/3)*(1/8)*k21a: R21b:=k21b*CH2DOH(t)*OH(t):
```
21c. CH2DOH + OH --> CHDOH + H2O
```
> k21c := (2/3)*k21a: R21c:=k21c*CH2DOH(t)*OH(t):
```
21d. CH3OH + OD --> CH2OH + HDO
```
> k21d := k21a: R21d:=k21d*CH3OH(t)*OD(t):
```
21e. CH2DOH + OD --> CHDOH + HDO
```
> k21e := (2/3)*k21a: R21e:=k21e*CH2DOH(t)*OD(t):
```
21f. CH2DOH + OD --> CH2OH + D2O
```
> k21f := (1/3)*(1/8)*k21a: R21f:=k21f*CH2DOH(t)*OD(t):
```
22a. CH2OH + O2 --> CH2O + HO2
```
> k22a := 9.6e-12: R22a:=k22a*CH2OH(t)*O2:
```
22b. CHDOH + O2 --> CHDO + HO2
```
> k22b := 9.6e-12: R22b:=k22b*CHDOH(t)*O2:
```
23. O3 + NO --> NO2
```
> k23 := 1.9e-14: R23:=k23*O3(t)*NO(t):
```
24a. CO + OH --> CO2 + HO2
```
> k24a := 2.3e-13: R24a:=k24a*CO(t)*OH(t):
```
24b. CO + OD --> CO2 + DO2
```
> k24b := 5.0e-14: R24b:=k24b*CO(t)*OD(t):
```
25a. H2 + OH --> H2O + HO2
```
> k25a := 6.7e-15: R25a:=k25a*H2(t)*OH(t):
```
25b. HD + OH --> H2O + DO2
```
> k25b := 2.5e-15: R25b:=k25b*HD(t)*OH(t):
```
25c. HD + OH --> HDO + HO2
```
> k25c := 6.7e-16: R25c:=k25c*HD(t)*OH(t):
```
25d. H2 + OD --> HDO + HO2
```
> k25d := 7.4e-15: R25d:=k25d*H2(t)*OD(t):
```
25e. HD + OD --> HDO + DO2
```
> k25e := 0.9*k25b: R25e:=k25e*HD(t)*OD(t):
```
25f. HD + OD --> D2O + HO2
```
> k25f := 0.9*k25c: R25f:=k25f*HD(t)*OD(t):
```
26. RO2 + RO2 --> 2RO
```
> k26 := 1.3e-14: R26:=k26*RO2(t)*RO2(t):
```
27. RO2 + RO2 --> RO + cC6H12
```
> k27 := 7.7e-14: R27:=k27*RO2(t)*RO2(t):
```
28a. RO2 + HO2 --> cC6H12
```
> k28a := 17.1e-12: R28a:=k28a*RO2(t)*HO2(t):
```
28b. RO2 + DO2 --> cC6H12
```
> k28b := k28a: R28b:=k28b*RO2(t)*DO2(t):
```
29. RO + O2 --> cC6H12 + HO2
```
> k29 := 2.0e-17: R29:=k29*RO(t)*O2:
```
30aa. HOCH2O2 + HO2 --> HOCH2OOH + O2
```
> k30aa := 6.0e-12: R30aa:=k30aa*HOCH2O2(t)*HO2(t):
```
30ab. HOCH2O2 + DO2 --> 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):
>
```
34a. PNA --> HO2 + NO2
```
> k34a := 10:R34a := k34a*PNA(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+R19c+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*R20m+R20n+1.5*R20o+
R20p+R22a+R22b+R24a+R25a+R25c+R25d+R25f-R28a+R29-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*R20
h+0.5*R20j+0.5*R20l+0.5*R20m+0.5*R20n+0.5*R20o+R20p+R24b+R2
5b+R25e-R28b-R30ab-R30ad-R30af-R30ah-R30bb-R30bd-R30bf-
R30bh-R30cb-R30cd-R30cf-R30ch+R33b+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-R21c-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-R21f-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+R30
be+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+
R25e+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-R34a, 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-R30cb-R33a,
HOCH2O2(0)=startconc:
> D_DOCH2O2:=diff(DOCH2O2(t),t) = R11b-R12b-R20c-R20g-R20i-
R20j-2*R20k-R20l-R20o-R30ac-R30ad-R30bc-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-R30be-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-R30bg-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*R
20h+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*
R20n+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+
R20p+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:
> D_mR34a:=diff(mR34a(t),t) = R34a, mR34a(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, D_mR34a]:
>
```

Solution and plotting

```
> with(plots):
Warning, the name changecoords has been redefined
```

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, 2262009590175448, 18064009, 44452500972406

21, 21, 2262016615263571, 3961788, 44449563509199

41, 41, 2262020780896112, 2865596, 44446304019080

61, 61, 2262023112351033, 2371058, 44442968899617

81, 81, 2262024696773336, 2073032, 44439627617103

101, 101, 2262025877189123, 1867568, 44436307425925

121, 121, 2262026806068759, 1714345, 44433020573319

141, 141, 2262027564281749, 1594040, 44429772751046

161, 161, 2262028199726625, 1496086, 44426566439695

181, 181, 2262028743020558, 1414148, 44423402433414

201, 201, 2262029214861098, 1344168, 44420280603313

221, 221, 2262029629861137, 1283407, 44417200305521

241, 241, 2262029998689748, 1229941, 44414160610591

261, 261, 2262030329363103, 1182371, 44411160436529

281, 281, 2262030628050157, 1139651, 44408198628286

301, 301, 2262030899583500, 1100982, 44405274006383

$j := 1$

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

1, 1105095147207160, 61342129088, 17523394457, 0

21, 1101342606662267, 3228128786872, 82118008411, 0

41, 1097322584207876, 6930832037933, 114839338462, 0

61, 1093241162126371, 10756916401221, 140119976958, 0

81, 1089166552336962, 14609046247262, 161468546123, 0

101, 1085125709026225, 18448871268766, 180265148937, 0

121, 1081130526094499, 22258613008691, 197223643711, 0

141, 1077186269579706, 26029483409335, 212771175877, 0

161, 1073294954111217, 29757153276297, 227188024945, 0

181, 1069456892247125, 33439687011047, 240670264065, 0

201, 1065671474873664, 37076499910111, 253361684212, 0

221, 1061937590933342, 40667792139218, 265371624119, 0

241, 1058253863982715, 44214224661531, 276785645297, 0

261, 1054618789407673, 47716726727103, 287672279183, 0

281, 1051030815496811, 51176378279468, 298087483874, 0

301, 1047488391902031, 54594336474535, 308077697576, 0

$j := 2$

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

1, 3998763, 65055388, 2845, 7113529592

21, 42775903, 2684237338, 632, 7112781136

41, 65850573, 5797980957, 457, 7111948725

61, 85654495, 9058593810, 379, 7111096659

81, 103742708, 12372701531, 331, 7110242881

101, 120716091, 15699498308, 298, 7109394426

121, 136878915, 19017734524, 274, 7108554461

141, 152409684, 22315294387, 255, 7107724461

161, 167423596, 25584919484, 239, 7106905070

181, 182000214, 28822163727, 226, 7106096500

201, 196197367, 32024309649, 215, 7105298722

221, 210058806, 35189750063, 205, 7104511575

241, 223618712, 38317614118, 196, 7103734823

261, 236904512, 41407531496, 189, 7102968191

281, 249938706, 44459477822, 182, 7102211385

301, 262740100, 47473669893, 176, 7101464104

```
> 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, 176837320546, 9609018, 133321555067, 5

21, 176209545979, 513561651, 638422142342, 6

41, 175551360687, 1104206269, 903586529690, 6

61, 174886230302, 1714863492, 1112667436539, 6

81, 174223726496, 2329833964, 1291902457691, 6

101, 173567638669, 2942927641, 1451620504289, 6

121, 172919599820, 3551270805, 1597178346838, 6

141, 172280290655, 4153439571, 1731792439226, 6

161, 171649926830, 4748729537, 1857581476823, 6

181, 171028483249, 5336822851, 1976033559311, 6

201, 170415806951, 5917620059, 2088244373602, 6

221, 169811677602, 6491148786, 2195050376137, 6

241, 169215841357, 7057511427, 2297108646093, 6

261, 168628030291, 7616854050, 2394947442747, 6

281, 168047973715, 8169347380, 2488999660168, 5

301, 167475404780, 8715174908, 2579625789576, 5

```
> 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, 30378371, 220308683, 7836302, 3

21, 328590015, 8159692925, 906136267, 10429

41, 509083701, 17523494844, 2565585504, 61448

61, 665636819, 27409747474, 4743258608, 173375

81, 809824218, 37542534339, 7335536942, 359828

101, 946072563, 47792418733, 10279341775, 630810

121, 1076599974, 58087231418, 13530909284, 994030

141, 1202694123, 68382750139, 17057558256, 1455608

161, 1325177572, 78650251939, 20833684206, 2020502

181, 1444612921, 88870368747, 24838534081, 2692790

201, 1561405414, 99029730281, 29054855206, 3475856

221, 1675859129, 109118990192, 33468020454, 4372534

241, 1788209931, 119131596172, 38065432762, 5385206

261, 1898645882, 129062990771, 42836103933, 6515880

281, 2007320444, 138910071364, 47770346746, 7766257

301, 2114361329, 148670812824, 52859543550, 9137772

```
> 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, 7188712, 1391759, 30378372, 220308684

21, 75749966, 2585266, 328590015, 8159692934

41, 116027893, 2620481, 509083701, 17523494858

61, 150361874, 2635416, 665636819, 27409747492

81, 181591588, 2644147, 809824219, 37542534361

101, 210827736, 2650030, 946072564, 47792418758

121, 238638456, 2654321, 1076599975, 58087231446

141, 265359566, 2657614, 1202694124, 68382750170

161, 291208827, 2660230, 1325177573, 78650251972

181, 316336923, 2662361, 1444612922, 88870368782

201, 340853290, 2664131, 1561405415, 99029730319

221, 364840447, 2665620, 1675859130, 109118990232

241, 388362510, 2666889, 1788209932, 119131596214

261, 411470538, 2667979, 1898645883, 129062990815

281, 434206027, 2668923, 2007320445, 138910071409

301, 456603298, 2669743, 2114361330, 148670812871

```
> 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, 118741, 8259303960, 0, 0

21, 8109578, 394536929, 0, 0

41, 18603906, 228547997, 0, 0

61, 30296502, 167546223, 0, 0

81, 42741086, 135029920, 0, 0

101, 55713484, 114485981, 0, 0

121, 69079464, 100164520, 0, 0

141, 82750383, 89519231, 0, 0

161, 96663879, 81241624, 0, 0

181, 110774085, 74586853, 0, 0

201, 125046138, 69097972, 0, 0

221, 139452842, 64478025, 0, 0

241, 153972552, 60525169, 0, 0

261, 168587741, 57096985, 0, 0

281, 183284025, 54089853, 0, 0

301, 198049456, 51426496, 0, 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, 0, 0

21, 0, 0, 0, 0

41, 0, 0, 0, 0

61, 0, 0, 0, 0

81, 0, 0, 0, 0

101, 0, 0, 0, 0

121, 0, 0, 1, 0

141, 0, 0, 1, 0

161, 0, 0, 1, 0

181, 0, 0, 1, 0

201, 0, 0, 1, 0

221, 0, 0, 1, 0

241, 0, 0, 1, 0

261, 0, 0, 1, 0

281, 0, 0, 1, 0

301, 0, 0, 1, 0

```
> 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, 410, 618255, 49238195705, 8433336095

21, 21581, 61929998, 1738128378232, 40148995674

41, 46335, 169263682, 3651166407934, 50752532992

61, 71914, 307393680, 5616469274832, 57656438938

81, 97668, 470526492, 7589258399278, 62750185791

101, 123341, 655253187, 9551946461181, 66750524067

121, 148813, 859239481, 11496539688268, 70015791210

141, 174027, 1080748438, 13419232390188, 72752926301

161, 198952, 1318417231, 15318276578362, 75092820356

181, 223576, 1571136417, 17193011530644, 77123678686

201, 247894, 1837978001, 19043377375497, 78907798822

221, 271909, 2118149475, 20869654378948, 80490808038

241, 295625, 2410962824, 22672315784758, 81907107994

261, 319048, 2715812764, 24451941964083, 83183259997

281, 342184, 3032160905, 26209168727212, 84340182314

301, 365043, 3359523925, 27944655404132, 85394628186

```
> 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, 38375897, 350419460, 2580501, 6841201588

21, 414141820, 13528167604, 262663664, 72569892398

41, 640784846, 29119456763, 724218514, 111555481632

61, 836945809, 45526935099, 1324327021, 144846974371

81, 1017309633, 62287937408, 2038923294, 175110985759

101, 1187504745, 79191415357, 2853740403, 203394829522

121, 1350357805, 96122700475, 3758935313, 230237819347

141, 1507513491, 113013338924, 4747131701, 255961343744

161, 1660024764, 129820090917, 5812503829, 280775680805

181, 1808613349, 146514696213, 6950280342, 304827715422

201, 1953800149, 163078349592, 8156447990, 328225156640

221, 2095976740, 179498490331, 9427561828, 351050007967

241, 2235447354, 195766824421, 10760616976, 373366597142

261, 2372454907, 211878053777, 12152958245, 395226631778

281, 2507197857, 227829027022, 13602214279, 416672524864

301, 2639841529, 243618152625, 15106248175, 437739662965

```
> 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, 434364352, 378875, 61268355930, 0

21, 1106005515, 112137713, 17446081724, 2

41, 1183436529, 354104985, 13391641204, 3

61, 1224396812, 680363134, 11263399763, 4

81, 1251451605, 1066319214, 9863317828, 5

101, 1271252562, 1496843481, 8842395837, 5

121, 1286637902, 1961832636, 8051792707, 6

141, 1299071993, 2454154299, 7414673615, 7

161, 1309405335, 2968564906, 6886421002, 7

181, 1318173859, 3501087850, 6438950625, 8

201, 1325736068, 4048632121, 6053512523, 8

221, 1332343008, 4608746450, 5717007307, 9

241, 1338176953, 5179454220, 5419955145, 9

261, 1343374190, 5759139081, 5155288987, 9

281, 1348039121, 6346463422, 4917609036, 10

301, 1352253378, 6940308756, 4702710360, 10

```
> 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, 1, 0, 0, 4

21, 1, 5, 6, 4

41, 2, 7, 9, 5

61, 2, 10, 12, 5

81, 2, 12, 14, 5

101, 2, 13, 16, 5

121, 2, 15, 18, 5

141, 2, 17, 20, 5

161, 2, 18, 22, 5

181, 2, 19, 23, 5

201, 2, 20, 25, 5

221, 1, 21, 26, 5

241, 1, 22, 28, 5

261, 1, 23, 29, 5

281, 1, 24, 30, 5

301, 1, 25, 31, 5

```
> 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, 0, 1, 6563, 146061303309

21, 1, 14, 345372, 656913025324

41, 1, 23, 741529, 900321743969

61, 1, 30, 1150898, 1082828297448

81, 1, 36, 1563066, 1234274138265

101, 1, 41, 1973929, 1366281984607

121, 1, 46, 2381585, 1484766258380

141, 1, 51, 2785092, 1593196766818

161, 1, 55, 3183988, 1693802033843

181, 1, 59, 3578065, 1788106966943

201, 1, 62, 3967259, 1877205425797

221, 1, 66, 4351593, 1961911225207

241, 2, 69, 4731135, 2042848045171

261, 2, 72, 5105986, 2120505327682

281, 2, 75, 5476260, 2195274932848

301, 2, 78, 5842082, 2267476172435

```
> 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, 4618479215, 6154719, 665957, 4940149

21, 36142619206, 1226105329, 143008, 6324515

41, 53048069857, 3161775409, 113510, 6652333

61, 65105633370, 5015197129, 100063, 6728388

81, 74502162888, 6486454388, 91909, 6715309

101, 82200828600, 7520548623, 86249, 6663425

121, 88720037839, 8176075420, 81994, 6593233

141, 94372585630, 8547549793, 78623, 6514381

161, 99362089171, 8725635992, 75852, 6431831

181, 103828571134, 8781764195, 73509, 6348279

201, 107872361746, 8766016594, 71487, 6265238

221, 111567831096, 8710707481, 69712, 6183566

241, 114971402854, 8635363340, 68133, 6103747

261, 118126999979, 8551146816, 66713, 6026044

281, 121069501036, 8464126905, 65424, 5950577

301, 123826894263, 8377442102, 64244, 5877388

```
> 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, 318, 108391588, 79151079, 446135959

21, 2488, 258838622, 1576658355, 1454869019

41, 3652, 291854729, 2650323062, 1564386575

61, 4482, 301336251, 3593308519, 1596001665

81, 5129, 301992232, 4453248786, 1600433630

101, 5659, 298723452, 5252361837, 1592844633

121, 6107, 293594082, 6003604409, 1579363241

141, 6497, 287591484, 6715485106, 1562885488

161, 6840, 281225693, 7394027814, 1544916880

181, 7148, 274772857, 8043725628, 1526290543

201, 7426, 268385912, 8668060671, 1507487089

221, 7680, 262149866, 9269811737, 1488790186

241, 7915, 256110183, 9851248092, 1470369626

261, 8132, 250289513, 10414257816, 1452325991

281, 8334, 244696828, 10960436229, 1434716031

301, 8524, 239332599, 11491148800, 1417570351

```
> 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, 27886688585, 30411777, 17500971591, 132884877384

21, 19852867407, 147894911, 82402209923, 625679980373

41, 15577717311, 208386004, 115697617642, 878492011348

61, 13214647303, 255644630, 141694676748, 1075887681279

81, 11625793034, 295950093, 163860806132, 1244195101803

101, 10452966243, 331762406, 183552842858, 1393716736765

121, 9537568000, 364348928, 201469348201, 1529756761932

141, 8795832762, 394465194, 218026582111, 1655475839092

161, 8178356496, 422605318, 233496683493, 1772940318966

181, 7653688898, 449113955, 248069423540, 1883591134221

201, 7200651812, 474243215, 261883587760, 1988482083213

221, 6804348676, 498184386, 275044459123, 2088412579540

241, 6453940626, 521086880, 287634259742, 2184006935704

261, 6141310906, 543070187, 299718734985, 2275764356287

281, 5860233811, 564231746, 311351492572, 2364091884706

301, 5605846148, 584652337, 322576968807, 2449326925815

```
> 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, 49295610535, 48405445071, 618255, 2580501

21, 1740109269932, 1708465864669, 61930020, 262663707

41, 3655468391965, 3588562928288, 169263804, 724218760

61, 5623253942203, 5519819922500, 307394019, 1324327704

81, 7598610915678, 7458263685349, 470527185, 2038924700

101, 9563915344565, 9386634690396, 655254390, 2853742855

121, 11511152813357, 11297095699078, 859241364, 3758939167

141, 13436504894346, 13185921378499, 1080751184, 4747137338

161, 15338215260743, 15051405815789, 1318421030, 5812511654

181, 17215617503191, 16892909561249, 1571141467, 6950290777

201, 19068647755471, 18710382098975, 1837984509, 8156461473

221, 20897583418361, 20504105976200, 2118157652, 9427578813

241, 22702895650333, 22274552429999, 2410972888, 10760637930

261, 24485163291465, 24022297200842, 2715824935, 12152983646

281, 26245021023769, 25747969874234, 3032175409, 13602244615

301, 27983127346866, 27452222618680, 3359540991, 15106283944

```
> 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, 206085, 1423185, 572843027, 79151079

21, 20643340, 144863014, 42457074830, 1576658355

41, 56421268, 399417619, 98203104302, 2650323062

61, 102464673, 730386794, 157749809585, 3593308519

81, 156842395, 1124497865, 218176139159, 4453248786

101, 218418130, 1573882423, 278287866290, 5252361837

121, 286413788, 2073111904, 337535241969, 6003604409

141, 360250395, 2618118168, 395657140306, 6715485106

161, 439473677, 3205688245, 452535756486, 7394027814

181, 523713822, 3833190670, 508129073336, 8043725628

201, 612661503, 4498412084, 562436614424, 8668060671

221, 706052551, 5199452557, 615480978973, 9269811737

241, 803657629, 5934654857, 667297423973, 9851248092

261, 905274978, 6702554615, 717927816077, 10414257816

281, 1010725136, 7501843998, 767417040999, 10960436229

301, 1119846997, 8331344476, 815810839119, 11491148800

```
> 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, 57999601, 7997533, 440617809, 60756804

21, 2117327196, 85551876, 16319398856, 657180571

41, 4510840566, 131701250, 35047016432, 1018168208

61, 7011797259, 171309123, 54819535841, 1331274668

81, 9553969515, 207485574, 75085123920, 1619649671

101, 12107690602, 241432363, 95584907154, 1892146554

121, 14657197159, 273758036, 116174547017, 2153201559

141, 17193324742, 304819595, 136765598968, 2405390034

161, 19710466901, 334847440, 157300617065, 2650357105

181, 22205103564, 364000697, 177740865156, 2889227972

201, 24675012945, 392395024, 198059602667, 3122813124

221, 27118817486, 420117920, 218238136889, 3351720717

241, 29535706691, 447237751, 238263363202, 3576422482

261, 31925260769, 473809372, 258126166702, 3797294544

281, 34287333974, 499877779, 277820342134, 4014643824

301, 36621974831, 525480584, 297341839245, 4228725751

```
> 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;
```

$$j := 19$$

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

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

$$21,\ 0,\ 0,\ 0,\ 0$$

$$41,\ 0,\ 0,\ 0,\ 0$$

$$61,\ 0,\ 0,\ 0,\ 0$$

$$81,\ 0,\ 0,\ 0,\ 0$$

$$101,\ 0,\ 0,\ 0,\ 0$$

$$121,\ 0,\ 0,\ 0,\ 0$$

$$141,\ 0,\ 0,\ 0,\ 0$$

$$161,\ 0,\ 0,\ 1,\ 0$$

$$181,\ 0,\ 0,\ 1,\ 0$$

$$201,\ 0,\ 0,\ 1,\ 0$$

$$221,\ 0,\ 0,\ 1,\ 0$$

$$241,\ 0,\ 0,\ 1,\ 0$$

$$261,\ 0,\ 0,\ 1,\ 0$$

281, 0, 0, 1, 0

301, 0, 0, 1, 0

```
> 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, 178232, 742531535, 46408221, 6398861

21, 6279043, 26161838111, 1635114882, 66546207

41, 13163664, 54849905687, 3428119105, 101130804

61, 20209042, 84210086178, 5263130386, 130191940

81, 27253853, 113569807848, 7098112991, 156300862

101, 34235586, 142668354021, 8916772126, 180471052

121, 41126538, 171390090065, 10711880629, 203225436

141, 47914139, 199682481094, 12480155068, 224876044

161, 54593204, 227523798022, 14220237376, 245627240

181, 61162411, 254908428628, 15931776789, 265621913

201, 67622541, 281839533567, 17614970848, 284964943

221, 73975535, 308325124980, 19270320311, 303736260

241, 80223968, 334375865032, 20898491565, 321998631

261, 86370745, 360003791195, 22500236950, 339802565

281, 92418913, 385221556710, 24076347294, 357189542

301, 98371559, 410041968266, 25627623017, 374194209

```
> 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, 102381776, 24575, 381078, 2010870

21, 1064739305, 255552, 57254279, 307030227

41, 1618092858, 388347, 167625996, 906923924

61, 2083071043, 499925, 313361997, 1707164872

81, 2500813793, 600162, 486082388, 2663413588

101, 2887536836, 692950, 680640235, 3748053718

121, 3251606984, 780298, 893485617, 4941797996

141, 3598016704, 863405, 1121998006, 6230247837

161, 3930035835, 943055, 1364152901, 7602165931

181, 4249950607, 1019799, 1618334070, 9048497593

201, 4559439093, 1094038, 1883218745, 10561768873

221, 4859780162, 1166079, 2157703099, 12135693521

241, 5151978094, 1236165, 2440851480, 13764903838

261, 5436841044, 1304488, 2731860594, 15444759630

281, 5715032670, 1371209, 3030033363, 17171208154

301, 5987107351, 1436460, 3334759347, 18940678570

```
> 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, 251359, 34706, 277649, 52617

21, 38378778, 1275200, 10201597, 1906534

41, 113365490, 2710107, 21680860, 4019123

61, 213395609, 4290495, 34323960, 6321862

81, 332926698, 5989445, 47915563, 8776943

101, 468506715, 7790316, 62322528, 11361276

121, 617724749, 9681146, 77449166, 14058417

141, 778780980, 11652690, 93221518, 16855749

161, 950270741, 13697485, 109579883, 19743161

181, 1131062199, 15809331, 126474644, 22712299

201, 1320221109, 17982962, 143863693, 25756111

221, 1516961690, 20213839, 161710716, 28868551

241, 1720612980, 22498000, 179984003, 32044363

261, 1930594954, 24831948, 198655581, 35278933

281, 2146401019, 27212570, 217700564, 38568174

301, 2367584821, 29637082, 237096655, 41908440

```
> 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, 8433355847, 434365365, 1391763, 19752

21, 40152271514, 1106113429, 2585540, 3275839

41, 50760833798, 1183670290, 2621039, 8300805

61, 57670693654, 1224762510, 2636262, 14254715

81, 62771041496, 1251952868, 2645283, 20855705

101, 66778474036, 1271891917, 2651454, 27949970

121, 70051230624, 1287417257, 2656036, 35439414

141, 72796182148, 1299992860, 2659619, 43255847

161, 75144169489, 1310468955, 2662527, 51349133

181, 77183359606, 1319381273, 2664949, 59680920

201, 78976019805, 1327088166, 2667010, 68220983

221, 80567752974, 1333840563, 2668792, 76944936

241, 81992940732, 1339820646, 2670352, 85832739

261, 83278127655, 1345164622, 2671734, 94867658

281, 84444217860, 1349976832, 2672969, 104035546

301, 85507952489, 1354338853, 2674082, 113324303

```
> 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, 1013, 2, 6561, 410

21, 107914, 82, 345290, 21581

41, 233761, 177, 741352, 46335

61, 365698, 275, 1150623, 71914

81, 501263, 374, 1562692, 97668

101, 639355, 472, 1973457, 123341

121, 779355, 570, 2381015, 148813

141, 920867, 666, 2784426, 174027

161, 1063620, 762, 3183226, 198952

181, 1207413, 856, 3577208, 223576

201, 1352098, 950, 3966309, 247894

221, 1497556, 1042, 4350551, 271909

241, 1643693, 1133, 4730003, 295625

261, 1790432, 1222, 5104764, 319048

281, 1937711, 1311, 5474949, 342184

301, 2085475, 1399, 5840683, 365043

```
> 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, 13236508, 44824725, 813564, 6180590

21, 643541280, 1954097731, 9971462, 76626865

41, 1408095657, 4253301510, 15637367, 120946424

61, 2206071948, 6672775692, 20484279, 159261890

81, 3013125837, 9140310785, 24889287, 194375621

101, 3819220319, 11623886176, 29002089, 227389724

121, 4619432504, 14106534535, 32899907, 258867578

141, 5411143631, 16578380250, 36628728, 289141778

161, 6192917388, 19033355505, 40218610, 318427981

181, 6963977262, 21467620230, 43690546, 346875689

201, 7723936580, 23878719212, 47059944, 374593914

221, 8472648409, 26265097745, 50338557, 401665353

241, 9210117170, 28625806530, 53535636, 428154781

261, 9936444426, 30960314134, 56658651, 454114286

281, 10651794362, 33268383016, 59713758, 479586686

301, 11356371110, 35549984819, 62706127, 504607837

```
> 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, 44824725, 151797655, 2755201, 20931102

21, 1954097731, 5937857681, 30835774, 236901739

41, 4253301510, 12852161377, 47871699, 370160257

61, 6672775692, 20188083067, 62566151, 486322563

81, 9140310785, 27732513992, 76033545, 593676017

101, 11623886176, 35384438496, 88704657, 695389404

121, 14106534535, 43086852292, 100797330, 793047260

141, 16578380250, 50804363863, 112439120, 887566906

161, 19033355505, 58513651714, 123712179, 979532541

181, 21467620230, 66198732875, 134673130, 1069342512

201, 23878719212, 73848365114, 145363053, 1157282902

221, 26265097745, 81454511679, 155812974, 1243567795

241, 28625806530, 89011379694, 166047103, 1328362845

261, 30960314134, 96514791939, 176084841, 1411799857

281, 33268383016, 103961760053, 185942093, 1493986202

301, 35549984819, 111350184752, 195632143, 1575011110

```
> 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, 813564, 2755201, 50017, 379980

21, 9971462, 30835774, 227585, 1741083

41, 15637367, 47871699, 269857, 2071650

61, 20484279, 62566151, 299344, 2304721

81, 24889287, 76033545, 323400, 2496475

101, 29002089, 88704657, 344390, 2664955

121, 32899907, 100797330, 363378, 2818299

141, 36628728, 112439120, 380942, 2960894

161, 40218610, 123712179, 397427, 3095380

181, 43690546, 134673130, 413061, 3223477

201, 47059944, 145363053, 428000, 3346371

221, 50338557, 155812974, 442357, 3464918

241, 53535636, 166047103, 456217, 3579756

261, 56658651, 176084841, 469645, 3691375

281, 59713758, 185942093, 482693, 3800162

301, 62706127, 195632143, 495402, 3906428

```
> 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, 6180590, 20931102, 379980, 2886699

21, 76626865, 236901739, 1741083, 13320328

41, 120946424, 370160257, 2071650, 15905369

61, 159261890, 486322563, 2304721, 17747644

81, 194375621, 593676017, 2496475, 19276104

101, 227389724, 695389404, 2664955, 20628481

121, 258867578, 793047260, 2818299, 21866837

141, 289141778, 887566906, 2960894, 23024545

161, 318427981, 979532541, 3095380, 24121670

181, 346875689, 1069342512, 3223477, 25171244

201, 374593914, 1157282902, 3346371, 26182227

221, 401665353, 1243567795, 3464918, 27161063

241, 428154781, 1328362845, 3579756, 28112550

261, 454114286, 1411799857, 3691375, 29040365

281, 479586686, 1493986202, 3800162, 29947394

301, 504607837, 1575011110, 3906428, 30835954

```
> 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, 21029, 5475532, 87608505, 6254438

21, 742194, 193252699, 3092043177, 201886279

41, 1558854, 405903776, 6494460419, 419471177

61, 2397636, 624324875, 9989198002, 642203340

81, 3239438, 843542132, 13496674115, 865393414

101, 4076764, 1061603793, 16985660687, 1087201545

121, 4906215, 1277624018, 20441984289, 1306799925

141, 5726176, 1491182103, 23858913653, 1523802775

161, 6535910, 1702085752, 27233372031, 1738040910

181, 7335144, 1910263267, 30564212271, 1949458969

201, 8123858, 2115709531, 33851352493, 2158063960

221, 8902179, 2318457063, 37095313003, 2363897746

241, 9670315, 2518559689, 40296955023, 2567021568

261, 10428519, 2716083023, 43457328363, 2767507066

281, 11177068, 2911098736, 46577579779, 2965430911

301, 11916247, 3103681027, 49658896430, 3160871516

```
> 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, 99688143, 3, 0, 0

21, 3217822299, 10366, 21, 33

41, 6685862086, 61177, 120, 190

61, 10235943649, 172722, 332, 530

81, 13793324382, 358602, 681, 1093

101, 17328679206, 628805, 1184, 1909

121, 20828813846, 991028, 1855, 3002

141, 24287579441, 1451381, 2706, 4393

161, 27702279346, 2014815, 3745, 6100

181, 31072031167, 2685400, 4981, 8136

201, 34396946583, 3466516, 6420, 10516

221, 37677692801, 4360989, 8069, 13250

241, 40915245914, 5371197, 9932, 16349

261, 44110747777, 6499147, 12014, 19821

281, 47265420408, 7746532, 14319, 23675

301, 50380513570, 9114787, 16851, 27917

```
> 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, 9, 1, 1, 0

41, 51, 3, 4, 1

61, 142, 6, 8, 2

81, 293, 12, 16, 4

101, 512, 19, 25, 7

121, 805, 29, 38, 10

141, 1177, 40, 53, 14

161, 1635, 54, 71, 19

181, 2181, 70, 93, 25

201, 2818, 88, 117, 31

221, 3551, 109, 145, 39

241, 4381, 132, 177, 47

261, 5312, 157, 211, 57

281, 6345, 185, 250, 67

301, 7482, 216, 291, 78

```
> 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, 14593780713, 2017144566, 10116324296, 0

21, 242849932575, 13536837753, 1499219438320, 4

41, 333705186178, 15312334732, 3326641532778, 7

61, 393736806569, 16267013576, 5229511890616, 9

81, 438333555985, 16902832991, 7151651633480, 11

101, 473504914458, 17370838382, 9071004566447, 13

121, 502298804340, 17736142212, 10977298098860, 15

141, 526490963509, 18032554737, 12865390701854, 16

161, 547211312457, 18279800684, 14732678756417, 17

181, 565224603094, 18490350465, 16577918417399, 19

201, 581072747162, 18672567427, 18400633627119, 20

221, 595153672499, 18832320066, 20200796765784, 21

241, 607768028676, 18973876425, 21978646656672, 22

261, 619148340494, 19100432110, 23734580920147, 23

281, 629477991609, 19214438024, 25469090050713, 24

301, 638904027740, 19317812383, 27182715859580, 25

```
> 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, 0, 0, 0, 1

21, 0, 0, 0, 13

41, 0, 0, 0, 22

61, 0, 0, 0, 29

81, 0, 0, 0, 35

101, 0, 0, 0, 40

121, 0, 0, 0, 45

141, 0, 0, 0, 49

161, 0, 0, 0, 54

181, 0, 0, 0, 57

201, 0, 0, 0, 61

221, 0, 0, 0, 64

241, 0, 0, 0, 68

261, 0, 0, 0, 71

281, 0, 0, 0, 73

301, 0, 0, 0, 76

```
> 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, 0, 0, 0, 0

21, 1, 1, 0, 3

41, 1, 1, 0, 4

61, 1, 1, 0, 6

81, 1, 1, 0, 7

101, 1, 1, 0, 8

121, 1, 1, 0, 9

141, 1, 1, 0, 10

161, 1, 1, 0, 10

181, 1, 1, 0, 11

201, 1, 1, 0, 12

221, 1, 1, 0, 13

241, 1, 1, 0, 13

261, 1, 1, 0, 14

281, 2, 2, 0, 14

301, 2, 2, 0, 15

```
> 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, 1

21, 0, 0, 0, 8

41, 0, 0, 0, 13

61, 0, 0, 0, 17

81, 0, 0, 0, 21

101, 0, 0, 0, 24

121, 0, 0, 0, 27

141, 0, 0, 0, 30

161, 0, 0, 0, 32

181, 0, 0, 0, 34

201, 0, 0, 0, 37

221, 0, 0, 0, 39

241, 0, 0, 0, 41

261, 0, 0, 0, 42

281, 0, 0, 0, 44

301, 0, 0, 0, 46

```
> 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, 0, 0, 0, 0

21, 0, 0, 0, 2

41, 1, 1, 0, 3

61, 1, 1, 0, 4

81, 1, 1, 0, 5

101, 1, 1, 0, 5

121, 1, 1, 0, 6

141, 1, 1, 0, 6

161, 1, 1, 0, 7

181, 1, 1, 0, 7

201, 1, 1, 0, 8

221, 1, 1, 0, 8

241, 1, 1, 0, 9

261, 1, 1, 0, 9

281, 1, 1, 0, 9

301, 1, 1, 0, 10

```
> 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, 0

21, 0, 0, 0, 5

41, 0, 0, 0, 9

61, 0, 0, 0, 11

81, 0, 0, 0, 14

101, 0, 0, 0, 16

121, 0, 0, 0, 18

141, 0, 0, 0, 20

161, 0, 0, 0, 21

181, 0, 0, 0, 23

201, 0, 0, 0, 24

221, 0, 0, 0, 26

241, 0, 0, 0, 27

261, 0, 0, 0, 28

281, 0, 0, 0, 29

301, 0, 0, 0, 30

```
> 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, 0, 0, 0, 378875

21, 0, 0, 0, 112137713

41, 0, 0, 0, 354104985

61, 0, 0, 0, 680363134

81, 0, 0, 0, 1066319214

101, 0, 0, 0, 1496843481

121, 0, 0, 0, 1961832636

141, 1, 1, 0, 2454154299

161, 1, 1, 0, 2968564906

181, 1, 1, 0, 3501087850

201, 1, 1, 0, 4048632121

221, 1, 1, 0, 4608746450

241, 1, 1, 0, 5179454220

261, 1, 1, 0, 5759139081

281, 1, 1, 0, 6346463422

301, 1, 1, 0, 6940308756

```
> 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, 5, 1211, 19379, 1

21, 8893, 2332348, 37317573, 257

41, 40538, 10612515, 169800236, 857

61, 97205, 25427282, 406836513, 1750

81, 178819, 46753880, 748062078, 2909

101, 284664, 74403874, 1190461986, 4314

121, 413818, 108136235, 1730179758, 5950

141, 565312, 147697396, 2363158333, 7804

161, 738189, 192837281, 3085396496, 9865

181, 931530, 243315912, 3893054586, 12123

201, 1144463, 298905937, 4782494997, 14570

221, 1376168, 359393306, 5750292893, 17197

241, 1625876, 424577056, 6793232891, 19998

261, 1892862, 494268715, 7908299440, 22965

281, 2176451, 568291531, 9092664489, 26094

301, 2476005, 646479637, 10343674198, 29377

```
> 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, 167, 2676, 129, 8

21, 67364, 1077828, 4262, 70

41, 224376, 3590023, 8825, 104

61, 457834, 7325337, 13487, 132

81, 760634, 12170148, 18175, 158

101, 1127703, 18043256, 22861, 182

121, 1555016, 24880250, 27529, 205

141, 2039206, 32627301, 32173, 227

161, 2577376, 41238011, 36787, 248

181, 3166973, 50671568, 41370, 268

201, 3805722, 60891555, 45919, 289

221, 4491570, 71865127, 50435, 308

241, 5222651, 83562415, 54917, 328

261, 5997255, 95956073, 59364, 347

281, 6813808, 109020930, 63778, 366

301, 7670857, 122733711, 68159, 384

```
> j:=41;
lhs(p(1)[4*j+1]),lhs(p(1)[4*j+2]),lhs(p(1)[4*j+3]);
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]));
end do;
```

$$j := 41$$

$$mR33c(t),\ mR33d(t),\ mR34a(t)$$

1, 436, 60, 464451439

21, 12973, 540, 42198236209

41, 26695, 804, 97911249572

61, 40829, 1028, 157448473334

81, 55164, 1232, 217874146927

101, 69600, 1424, 277989142838

121, 84084, 1608, 337241647887

141, 98582, 1785, 395369548822

161, 113073, 1958, 452254530793

181, 127540, 2127, 507854300480

201, 141975, 2293, 562168228512

221, 156368, 2457, 615218829107

241, 170714, 2618, 667041313790

261, 185010, 2776, 717677526564

281, 199251, 2934, 767172344171

301, 213437, 3089, 815571506520

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Comments: