

**ISSA (ITERATIVE SCREENING AND STRUCTURE ANALYSIS) – A NEW REDUCTION METHOD
AND ITS APPLICATION TO THE TROPOSPHERIC CLOUD CHEMICAL MECHANISM RACM /
CAPRAM2.4**

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ELECTRONIC SUPPLEMENTARY MATERIAL (ESM)

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# === Liquid-phase part (reduced CAPRAM2.4) of the reduced
# === multiphase reaction mechanism CAPRAM2.4 + RACM.
# === Reduction according to: Mauersberger, G., 2005. ISSA (Iterative Screening
# === and Structure Analysis) – a new reduction method and its application
# === to the tropospheric cloud chemical mechanism RACM / CAPRAM2.4.
# === Atmospheric Environment, Special Issue Aerosol-cloud interaction:
# === Ground based hill capped cloud experiments and model development.
# ===
```

COMMENT All names of non-ionic aqueous phase species begin with a, cations end
COMMENT with p and anions end with m, respectively.

COMMENT CLASS: HENRY, TYPE: TEMP3

COMMENT Phase transfer

COMMENT $K_h = A \exp(B(1/T - 1/298))$

COMMENT $B = dH/R [K]$

CLASS: HENRY

CO2 = aCO2

TEMP3: A: 3.1e-2 B: 2423.0

CLASS: HENRY

O3 = aO3

TEMP3: A: 1.14e-2 B: 2300.0

CLASS: HENRY

HO2 = aHO2

TEMP3: A: 9.0e3 B: 0.0

CLASS: HENRY

HO = aHO

TEMP3: A: 25.0 B: 5280.0

CLASS: HENRY

H2O2 = aH2O2

TEMP3: A: 1.02e5 B: 6340.0

CLASS: HENRY

NO2 = aNO2

TEMP3: A: 1.2e-2 B: 1263.0

CLASS: HENRY

HONO = aHONO

TEMP3: A: 49.0 B: 4880.0

CLASS: HENRY

HNO3 = aHNO3

TEMP3: A: 2.1e5 B: 8700.0

CLASS: HENRY

NO3 = aNO3

TEMP3: A: 6.0e-1 B: 0.0

CLASS: HENRY

N2O5 = aN2O5

TEMP3: A: 1.4e0 B: 0.0

CLASS: HENRY

NH3 = aNH3

TEMP3: A: 60.7 B: 3920.0

CLASS: HENRY

HCL = aHCL

TEMP3: A: 1.1 B: 2020.0

CLASS: HENRY

HCHO = aHCHO

TEMP3: A: 2.5 B: 7216.0

CLASS: HENRY

ORA1 = aORA1

TEMP3: A: 5.53e3 B: 5630.0

CLASS: HENRY

SO2 = aSO2

TEMP3: A: 1.24 B: 3247.0

CLASS: HENRY

OP1 = aOP1

TEMP3: A: 310.0 B: 5607.0

CLASS: HENRY

PAA = aPAA

TEMP3: A: 6.69e2 B: 5890.0

CLASS: HENRY

MO2 = aMO2

TEMP3: A: 310.0 B: 5607.0

CLASS: HENRY

ETHPX = aETHPX

TEMP3: A: 340.0 B: 87.0

CLASS: HENRY

ETOH = aETOH

TEMP3: A: 1.9e2 B: 6290.0

CLASS: HENRY

CH3OH = aCH3OH

TEMP3: A: 2.2e2 B: 5390.0

CLASS: HENRY

SULF = aSULF

TEMP3: A: 8.7e11 B: 0.0

CLASS: HENRY

HNO4 = aHNO4

TEMP3: A: 3e4 B: 0.0

CLASS: HENRY

ACO3 = aACO3

TEMP3: A: 6.69e2 B: 5893.0

CLASS: HENRY

GLY = aGLY

TEMP3: A: 1.4 B: 0.0

CLASS: HENRY

[O2] = aO2

TEMP3: A: 1.3e-3 B: 1700.0

COMMENT --- THERE ARE xx AQUEOUS REACTIONS IN THE WET REACTION SCHEME;

CLASS: AQUA

FEOHpp = FEpp + aHO

PHOTABC: A: 4.76e-03 B: 2.19894e+00 C: 0.76087e+00

CLASS: AQUA

NO3m = aNO2 + aHO + OHm

PHOTABC: A: 4.57e-7 B: 2.59408e+00 C: 0.77213e+00

CLASS: AQUA

aH2O2 = aHO + aHO

PHOTABC: A: 7.64e-06 B: 2.46425e+00 C: 0.76355e+00

CLASS: AQUA

FEC2O42m = FEpp + C2O4mm + aCO2 + CO2m

PHOTABC: A: 2.47e-2 B: 1.95825e+00 C: 0.76782e+00

CLASS: AQUA



TEMP3: A: 50.0 B: 0.0

CLASS: AQUA



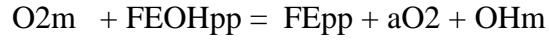
TEMP3: A: 2800.0 B: 0.0

CLASS: AQUA



TEMP3: A: 7.0e3 B: 0.0

CLASS: AQUA



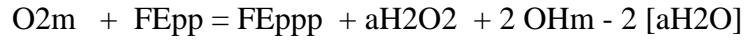
TEMP3: A: 1.5e8 B: 0.0

CLASS: AQUA



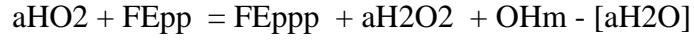
TEMP3: A: 1.5e8 B: 0.0

CLASS: AQUA



TEMP3: A: 1.0e7 B: 0.0

CLASS: AQUA



TEMP3: A: 1.2e6 B: -5050.0

CLASS: AQUA



TEMP3: A: 4.3e8 B: -1100.0

CLASS: AQUA



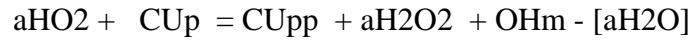
TEMP3: A: 1.0e7 B: 0.0

CLASS: AQUA



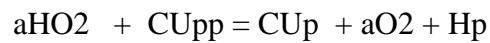
TEMP3: A: 1e10 B: 0.0

CLASS: AQUA



TEMP3: A: 2.3e9 B: 0.0

CLASS: AQUA



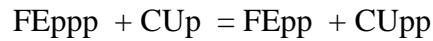
TEMP3: A: 1.0e8 B: 0.0

CLASS: AQUA



TEMP3: A: 8.0e9 B: 0.0

CLASS: AQUA



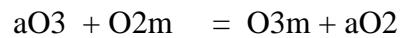
TEMP3: A: 1.3e7 B: 0.0

CLASS: AQUA



TEMP3: A: 1.3e7 B: 0.0

CLASS: AQUA



TEMP3: A: 1.5e9 B: -2200.0

CLASS: AQUA



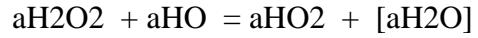
TEMP3: A: 330.0 B: -4500.0

CLASS: AQUA



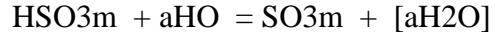
TEMP3: A: 4.85e7 B: -1060.0

CLASS: AQUA



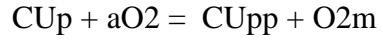
TEMP3: A: 3.0e7 B: -1680.0

CLASS: AQUA



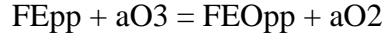
TEMP3: A: 2.7e9 B: 0.0

CLASS: AQUA



TEMP3: A: 4.6e5 B: 0.0

CLASS: AQUA



TEMP3: A: 8.2e5 B: -4690.0

CLASS: AQUA



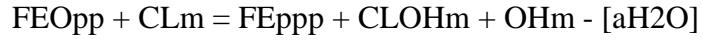
TEMP3: A: 9500.0 B: -2766.0

CLASS: AQUA



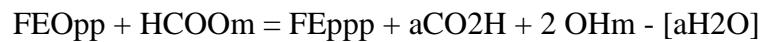
TEMP3: A: 2.5e5 B: 0.0

CLASS: AQUA



TEMP3: A: 100.0 B: 0.0

CLASS: AQUA



TEMP3: A: 3e5 B: 0.0

CLASS: AQUA



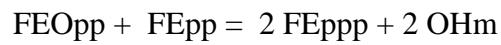
TEMP3: A: 2.5e3 B: 0.0

CLASS: AQUA



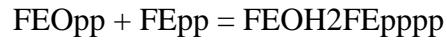
TEMP3: A: 400.0 B: -5352.0

CLASS: AQUA



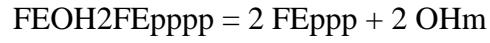
TEMP3: A: 7.2e4 B: -842.0

CLASS: AQUA



TEMP3: A: 1.8e4 B: -5052.0

CLASS: AQUA



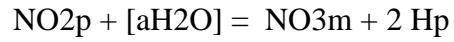
TEMP3: A: 0.49 B: -8780.0

CLASS: AQUA



TEMP3: A: 1e9 B: 0.0

CLASS: AQUA



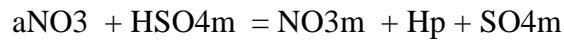
TEMP3: A: 8.9e7 B: 0.0

CLASS: AQUA



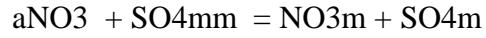
TEMP3: A: 4.9e6 B: -2000.0

CLASS: AQUA



TEMP3: A: 2.6e5 B: 0.0

CLASS: AQUA



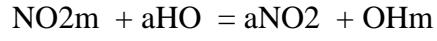
TEMP3: A: 1e5 B: 0.0

CLASS: AQUA



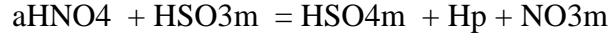
TEMP3: A: 4.5e-2 B: 0.0

CLASS: AQUA



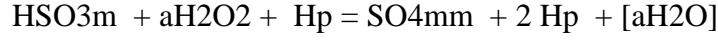
TEMP3: A: 9.1e9 B: 0.0

CLASS: AQUA



TEMP3: A: 3.3e5 B: 0.0

CLASS: AQUA



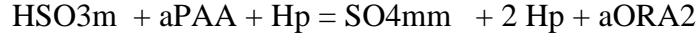
TEMP3: A: 7.2e7 B: -4000.0

CLASS: AQUA



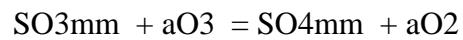
TEMP3: A: 1.7e7 B: -3800.0

CLASS: AQUA



TEMP3: A: 5.6e7 B: -3990.0

CLASS: AQUA



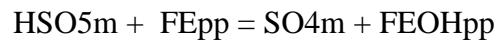
TEMP3: A: 1.5e9 B: -5280.0

CLASS: AQUA



TEMP3: A: 2.65e7 B: -5809.0

CLASS: AQUA



TEMP3: A: 3.0e4 B: 0.0

CLASS: AQUA



TEMP3: A: 1e10 B: 0.0

CLASS: AQUA



TEMP3: A: 4.6e9 B: 2165.0

CLASS: AQUA



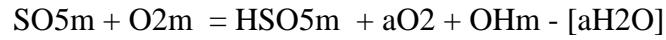
TEMP3: A: 2.2e8 B: -2600.0

CLASS: AQUA



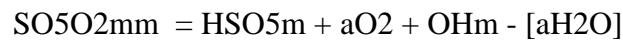
TEMP3: A: 1.7e9 B: 0.0

CLASS: AQUA



TEMP3: A: 2.34e8 B: 0.0

CLASS: AQUA



TEMP3: A: 1.2e3 B: 0.0

CLASS: AQUA



TEMP3: A: 2.5e9 B: 0.0

CLASS: AQUA



TEMP3: A: 5.8e8 B: 0.0

CLASS: AQUA



TEMP3: A: 1.7e7 B: 0.0

CLASS: AQUA



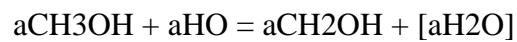
TEMP3: A: 11.0 B: -1110.0

CLASS: AQUA



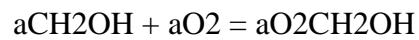
TEMP3: A: 7.14e6 B: 0.0

CLASS: AQUA



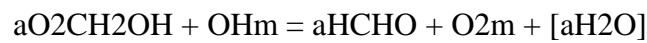
TEMP3: A: 1.0e9 B: -580.0

CLASS: AQUA



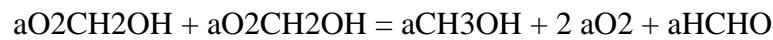
TEMP3: A: 2e9 B: 0.0

CLASS: AQUA



TEMP3: A: 1.65e10 B: 0.0

CLASS: AQUA



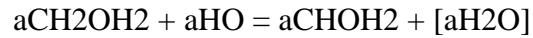
TEMP3: A: 1.05e9 B: 0.0

CLASS: AQUA



TEMP3: A: 2.1e9 B: -1200

CLASS: AQUA



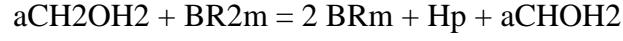
TEMP3: A: 1.0e9 B: -1020.0

CLASS: AQUA



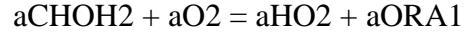
TEMP3: A: 1.4e7 B: -1300.0

CLASS: AQUA



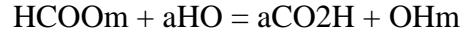
TEMP3: A: 3.0e3 B: 0.0

CLASS: AQUA



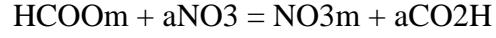
TEMP3: A: 2e9 B: 0.0

CLASS: AQUA



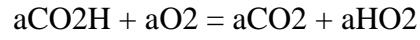
TEMP3: A: 3.2e9 B: -1000.0

CLASS: AQUA



TEMP3: A: 5.1e7 B: -2200.0

CLASS: AQUA



TEMP3: A: 2e9 B: 0.0

CLASS: AQUA



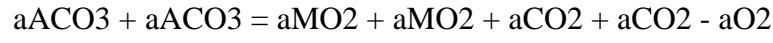
TEMP3: A: 7.4e7 B: -2200.0

CLASS: AQUA



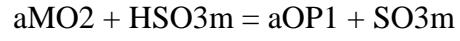
TEMP3: A: 3.6e7 B: -2200.0

CLASS: AQUA



TEMP3: A: 1.5e8 B: 0.0

CLASS: AQUA



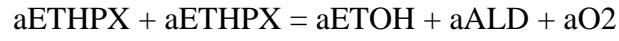
TEMP3: A: 5.0e5 B: 0.0

CLASS: AQUA



TEMP3: A: 1.0e8 B: 750.0

CLASS: AQUA



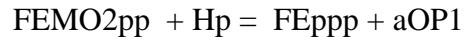
TEMP3: A: 6e7 B: 750.0

CLASS: AQUA



TEMP3: A: 8.6e5 B: 0.0

CLASS: AQUA



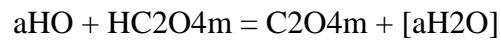
TEMP3: A: 3e4 B: 0.0

CLASS: AQUA



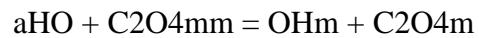
TEMP3: A: 100.0 B: 0.0

CLASS: AQUA



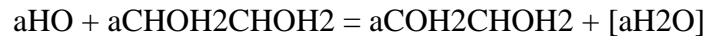
TEMP3: A: 1.9e8 B: -2800

CLASS: AQUA



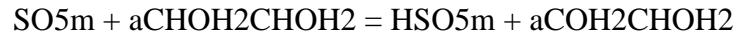
TEMP3: A: 1.6e8 B: -4300

CLASS: AQUA



TEMP3: A: 1.1e9 B: -1516.0

CLASS: AQUA



TEMP3: A: 5e5 B: 0.0

CLASS: AQUA



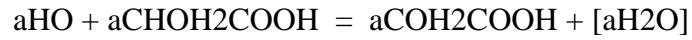
TEMP3: A: 1.38e9 B: 0.0

CLASS: AQUA



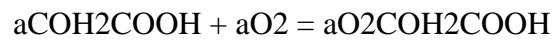
TEMP3: A: 1e7 B: 0.0

CLASS: AQUA



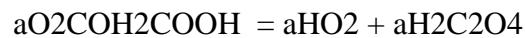
TEMP3: A: 3.6e8 B: -1000.0

CLASS: AQUA



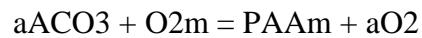
TEMP3: A: 2e9 B: 0.0

CLASS: AQUA



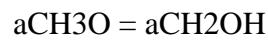
TEMP3: A: 2e9 B: 0.0

CLASS: AQUA



TEMP3: A: 1e9 B: 0.0

CLASS: AQUA



TEMP3: A: 1e6 B: 0.0

CLASS: AQUA



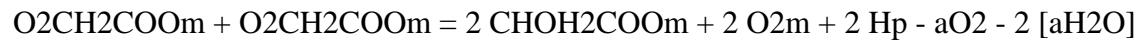
TEMP3: A: 2e7 B: 0.0

CLASS: AQUA



TEMP3: A: 1.88e7 B: 0.0

CLASS: AQUA



TEMP3: A: 7.5e6 B: 0.0

CLASS: AQUA



TEMP3: A: 2e7 B: -4090.0

CLASS: AQUA



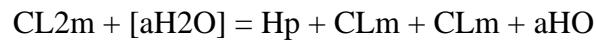
TEMP3: A: 3e5 B: 0.0

CLASS: AQUA



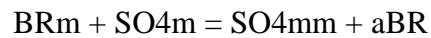
TEMP3: A: 2.1e5 B: 0.0

CLASS: AQUA



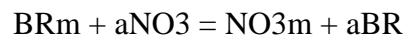
TEMP3: A: 23.4 B: 0.0

CLASS: AQUA



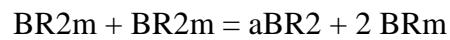
TEMP3: A: 2.1e9 B: 0.0

CLASS: AQUA



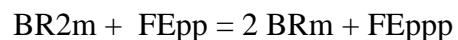
TEMP3: A: 3.8e9 B: 0.0

CLASS: AQUA



TEMP3: A: 1.7e9 B: 0.0

CLASS: AQUA



TEMP3: A: 3.6e6 B: -3330.0

CLASS: AQUA



TEMP3: A: 6.3e6 B: -4330.0

CLASS: AQUA



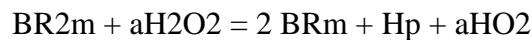
TEMP3: A: 3e5 B: 0.0

CLASS: AQUA



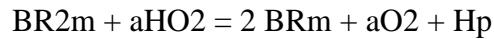
TEMP3: A: 2.2e5 B: 0.0

CLASS: AQUA



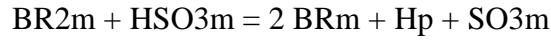
TEMP3: A: 1.0e5 B: 0.0

CLASS: AQUA



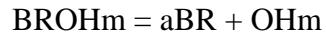
TEMP3: A: 6.5e9 B: 0.0

CLASS: AQUA



TEMP3: A: 5.0e7 B: -780.0

CLASS: AQUA



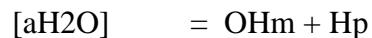
TEMP3: A: 4.2e6 B: 0.0

COMMENT --- THERE ARE 20 EQUILIBRIUM REACTIONS IN THE DISS REACTION SCHEME;

COMMENT --- B parameter is given as - delE/R attention (change to MM notation)!!!

COMMENT --- --> $K_e = A \exp(B(1/T - 1/298))$

CLASS: DISS



DTEMP: A: 1.8e-16 B: -6800.0 C: 1.3e11

COMMENT--- CLASS: DISS TYPE: DTEMP

COMMENT--- $\text{aCO}_2 + [\text{aH}_2\text{O}] = \text{aH}_2\text{CO}_3$

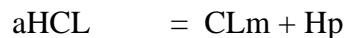
COMMENT--- PARAMETER: A: 7.7e-07 B: -9250.0 C: 5.60e+04

CLASS: DISS



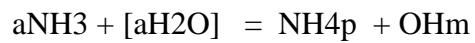
DTEMP: A: 4.3e-7 B: -913 C: 5.6e4

CLASS: DISS



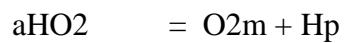
DTEMP: A: 1.72e+6 B: 6890.0 C: 2.9e5

CLASS: DISS



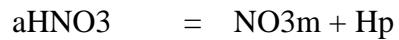
DTEMP: A: 3.17e-7 B: -560.0 C: 3.4e10

CLASS: DISS



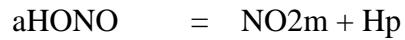
DCONST: A: 1.6e-5 B: 5.0e10

CLASS: DISS



DTEMP: A: 22.0 B: 1800.0 C: 5.0e10

CLASS: DISS



DTEMP: A: 5.3e-4 B: -1760.0 C: 5.0e10

CLASS: DISS



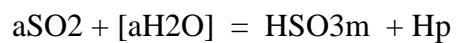
DCONST: A: 1.0e-5 B: 5.0e10

CLASS: DISS



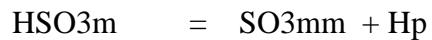
DCONST: A: 2.2e9 B: 4.6e-3

CLASS: DISS



DTEMP: A: 3.13e-4 B: 1940.0 C: 2.0e8

CLASS: DISS



DTEMP: A: 6.22e-8 B: 1960.0 C: 5.0e10

CLASS: DISS



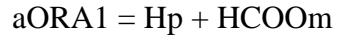
DCONST: A: 1000.0 B: 5e10

CLASS: DISS



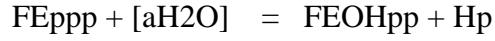
DTEMP: A: 1.02e-2 B: 2700.0 C: 1e11

CLASS: DISS



DTEMP: A: 1.77e-4 B: 12 C: 5e10

CLASS: DISS



DCONST: A: 1.1e-4 B: 4.3e8

CLASS: DISS



DCONST: A: 1.4e-7 B: 8.0e9

CLASS: DISS



DTEMP: A: 36.0 B: 4030.0 C: 5.1e-3

CLASS: AQUA



TEMP3: A: 2.5e+7 B: -2752.0

CLASS: AQUA



TEMP3: A: 3.79e-3 B: -5290.0

CLASS: DISS



DCONST: A: 1.4e5 B: 6e4

CLASS: DISS



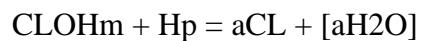
DCONST: A: 6.32e5 B: 1.9e4

CLASS: DISS



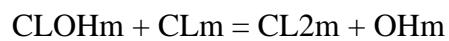
DCONST: A: 0.7 B: 6.1e9

CLASS: DISS1



DCONST: A: 5.1e6 B: 4100.0

CLASS: DISS



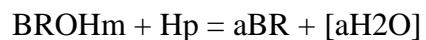
DCONST: A: 2.2e-4 B: 4.5e7

CLASS: DISS



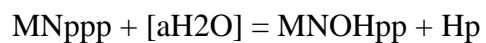
DCONST: A: 333.0 B: 3.3e7

CLASS: DISS1



DCONST: A: 1.8e12 B: 2.45e-2

CLASS: DISS



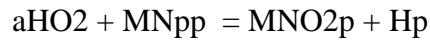
DCONST: A: 0.93 B: 2e10

CLASS: DISS



DCONST: A: 2.3e4 B: 6500.0

CLASS: DISS



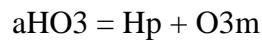
DCONST: A: 0.17 B: 6.5e6

CLASS: DISS



DCONST: A: 1e-5 B: 2e10

CLASS: DISS1



DCONST: A: 6.3e-9 B: 5.2e+10

CLASS: DISS



DCONST: A: 1.5e-5 B: 5e10

CLASS: DISS



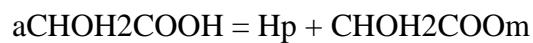
DCONST: A: 6.25e-5 B: 5.0e10

CLASS: DISS



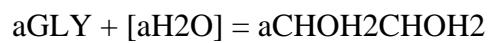
DCONST: A: 6.4e-2 B: 5.0e10

CLASS: DISS



DCONST: A: 3.16e-4 B: 2e10

CLASS: DISS



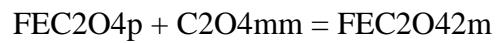
DCONST: A: 3900.0 B: 5.5e-3

CLASS: DISS



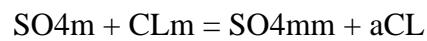
DCONST: A: 2.9e9 B: 3e-3

CLASS: DISS



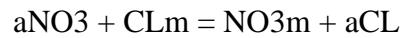
DCONST: A: 6.3e6 B: 3e-3

CLASS: DISS



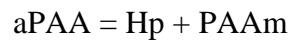
DCONST: A: 1.2 B: 2.1e8

CLASS: DISS



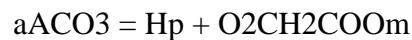
DTEMP: A: 3.4 B: -4300.0 C: 1e8

CLASS: DISS



DCONST: A: 6.3e-9 B: 5e10

CLASS: DISS



DTEMP: A: 1.75e-5 B: 46.0 C: 5e10

COMMENT---- CLASS: DISS TYPE: DTEMP

COMMENT---- aETHPX = Hp + CH₂OHCOOm

COMMENT---- PARAMETER: A: 1.75e-5 B: 46.0 C: 5e10