



## Input Files for Computer Simulation of Water Radiolysis

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# **Input Files for Computer Simulation of Water Radiolysis**

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April 1984**

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INPUT FILES FOR COMPUTER SIMULATION OF WATER RADIOLYSIS

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Abstract. This report contains radiation chemistry input files for CHEMSIMUL, a program package for numerical simulation of chemical reaction systems.

INIS-descriptors: CARBONATES; CHEMICAL REACTION KINETICS; CHLORIDES; COMPUTERIZED SIMULATION; G VALUE; IRON COMPOUNDS; RADIOLYSIS; WATER

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## 1. INTRODUCTION

Over the years we have constructed a series of input files for computer-simulation (1) of water radiolysis experiments. These files have proved adequate for simulation of our experimental results. The files are continuously objects for revisions as reactions and rate constants become better known.

The reaction equations are numbered in succession in order to facilitate addition of files. The rate constants are written after each equation separated with ";". The unit for the rate constant derives from the left-hand side of the equation. If there is only one reactant the unit is  $s^{-1}$ , if there are two the unit is  $dm^3mol^{-1}s^{-1}$ . If the two reactants are identical the rate constant is given as  $1k$ .

In order to preserve the mass, the water concentration is included in the computations and reactions with water are second-order reactions.

Note that  $E[-]$  symbolize one electron plus one water molecule. Where no reference is given the rate constants are chosen from the NBS-tables (2,3,4,5,6).

The G-value files are constructed with a complete preservation of mass and charge:

Hydrogen balance

$$-G(H_2O) = 0.5 * G(OH) + 0.5 * G(H) + G(H_2) + G(H_2O_2) + 0.5 * G(H[+]) + 0.5 * G(OH[-]) + G(E[-])$$

Oxygen balance

$$-G(H_2O) = G(OH) + 2G(H_2O_2) + G(OH[-]) + G(E[-])$$

Charge balance

$$G(H[+]) = G(E[-]) + G(OH[-])$$

## 2. WATER REACTIONS

FILENAME=EB/WATER

This file contains reactions for simulation of radiolysis of acid, neutral and alkaline water.

### References and notes

RE1:OH+OH=H2O2;6E9  
RE2:OH+E[-]=OH[-]+H2O;2.5E10  
RE3:H+H=H2O;2.5E10  
RE4:OH+O[-]=HO2[-];1.8E10  
RE5:OH+HO2=H2O3;7.9E9  
RE6:OH+O2[-]=OH[-]+O2;E10  
RE7:OH+O3[-]=O3+OH[-];2.5E9 (7)  
RE8:OH+O3[-]=HO2+O2[-];6E9 (7)  
RE9:OH+H2O2=H2O+O2[-]+H[+];2.7E7  
RE10:OH+HO2[-]=H2O+O2[-];7.5E9 (8)  
RE11:OH+OH[-]=O[-]+H2O;1.4E10  
RE12:OH+H2=H2O+H;4E7  
RE13:OH+O3=O2[-]+O2+H[+];E8 (9)  
RE19:E[-]+E[-]=2\*OH[-]+H2;3E9  
RE20:E[-]+H=OH[-]+H2;2E10  
RE21:E[-]+O[-]=2\*OH[-];1.5E10  
RE22:E[-]+O2[-]=HO2[-]+OH[-];1.2E10  
RE23:E[-]+H2O2=OH+OH[-]+H2O;1.6E10  
RE24:E[-]+HO2[-]=O[-]+OH[-]+H2O;3.5E9  
RE25:E[-]+H[+]=H+H2O;2.2E10  
RE26:E[-]+O2=O2[-]+H2O;2E10  
RE27:E[-]+O3=O3[-]+H2O;3.6E10 (10)  
RE28:E[-]+N2O=O[-]+N2+H2O;9E9  
RE31:H+H=H2;E10  
RE32:H+HO2=H2O2;2E10  
RE33:H+O2[-]=HO2[-];2E10  
RE34:H+H2O2=OH+H2O;6E7  
RE35:H+OH[-]=E[-];1.5E7  
RE36:H+O2=O2[-]+H[+];2E10  
RE37:H+O3=OH+O2;3.6E10 (10)



RE38:  $H+O[-]-OH[-]$ ; 2E10  
RE43:  $O[-]+O[-]-O2[-]$ ; 9E8  
RE44:  $O[-]+O2[-]-O3[-]$ ; 3.5E8 (11)  
RE45:  $O[-]+O3[-]-2*O2[-]$ ; 3.5E8 (11)  
RE46:  $O[-]+H2O2=O2[-]+H2O$ ; 5E8 (8)  
RE47:  $O[-]+HO2[-]=OH[-]+O2[-]$ ; 3.5E8 (8)  
RE48:  $O[-]+H2O=OH+OH[-]$ ; 2E6  
RE49:  $O[-]+O2=O3[-]$ ; 3.0E9  
RE50:  $O[-]+H2=OH[-]+H$ ; 2E8 (12)  
RE56:  $HO2=O2[-]+H[+]$ ; 8E5  
RE57:  $HO2+HO2=O2+H2O2$ ; 7.5E5  
RE58:  $HO2+O2[-]=O2+HO2[-]$ ; E8  
RE61:  $O2[-]+H[+]=HO2$ ; 5E10  
RE62:  $O2[-]+O3=O3[-]+O2$ ; 1.5E9 (10)  
RE64:  $H2O3=O2+H2O$ ; 2.1 (13)  
RE65:  $O3[-]=O[-]+O2$ ; 3.3E3 (14)  
RE66:  $O3[-]+H[+]=OH+O2$ ; 9E10 (7)  
RE68:  $H2O2+OH[-]=HO2[-]+H2O$ ; 5E8  
RE69:  $HO2[-]+H2O=H2O2+OH[-]$ ; 5.735E4  
RE70:  $HO2[-]+O3=O3[-]+O2[-]+H[+]$ ; 3E6 (15)  
RE73:  $H2O=H[+]+OH[-]$ ; 2.599E-5  
RE74:  $H2O+O2[-]=HO2[-]+OH[-]$ ; E8 (a)  
RE75:  $H2O+O3[-]=O2+2*OH[-]$ ; E8 (a)  
RE76:  $H[+]+OH[-]=H2O$ ; 1.43E11

Notes:

(a) Balance reactions of no significance for the kinetics.

### 3. CARBONATE REACTIONS

FILENAME=EB/CARBONATE

This file contains reactions that are used for simulation of radiolysis of carbonate in aqueous solution when combined with EB/WATER.

#### References and notes

RE80:OH+CO3[--]=CO3[-]+OH[-];4E8	
RE81:OH+HCO3[-]=CO3[-]+H2O;1.5E7	
RE82:O2[-]+CO3[-]=CO3[--]+O2;3.2E8	(a)
RE83:H2O2+CO3[-]=CO3[--]+O2[-]+2*H[+];4.3E5	(a)
RE84:HO2[-]+CO3[-]=CO3[--]+O2[-]+H[+];3E7	(a)
RE85:O3[-]+CO3[-]=CO3[--]+O3;6E7	(16)
RE86:H[+]+HCO3[-]=CO2+H2O;E10	(b)
RE87:OH[-]+HCO3[-]=CO3[--]+H2O;E9	(c)
RE88:H2O+CO2=HCO3[-]+H[+];70	(b)
RE89:H2O+CO3[--]=HCO3[-]+OH[-];3.6E3	(c)
RE90:H2O+CO4[--]=HO2[-]+OH[-]+CO2;0.2	(a)
RE91:CO3[-]+CO3[-]=CO4[--]+CO2;7E6	

#### Notes:

- (a) K.Sehested, to be published.
- (b)  $pK(CO2/HCO3[-]) = 6.4$ .
- (c)  $pK(HCO3[-]/CO3[--]) = 10.3$ .

#### 4. FERROUS REACTIONS

FILENAME=EB/FE

This file contains reactions that are used for simulation of radiolysis of ferrous/ferric in acid aqueous solution when combined with EB/WATER.

#### References and notes

RE105:  $\text{FE}^{++} + \text{OH} = \text{FE}^{+++} + \text{OH}^-$ ; 3.4E8  
RE106:  $\text{FE}^{++} + \text{E}^- = \text{FE}^{+++} + \text{OH}^- + \text{H}^-$ ; 1.2E8  
RE107:  $\text{FE}^{+++} + \text{E}^- = \text{FE}^{++} + \text{H}_2\text{O}$ ; 2E10  
RE108:  $\text{FE}^{++} + \text{H} = \text{FE}^{+++} + \text{H}^-$ ; 1.3E7  
RE109:  $\text{FE}^{+++} + \text{H} = \text{FE}^{++} + \text{H}^+$ ; 1E8  
RE110:  $\text{FE}^{++} + \text{HO}_2 = \text{FE}^{+++} + \text{HO}_2^-$ ; 1.6E6  
RE111:  $\text{FE}^{++} + \text{O}_2^- = \text{FE}^{+++} + \text{O}_2^{--}$ ; 2E8 (a)  
RE112:  $\text{FE}^{+++} + \text{O}_2^- = \text{FE}^{++} + \text{O}_2$ ; 5E8 (a)  
RE113:  $\text{FE}^{++} + \text{H}_2\text{O}_2 = \text{FE}^{+++} + \text{OH} + \text{OH}^-$ ; 62 (17)  
RE114:  $\text{FE}^{++} + \text{H}_2\text{O}_3 = \text{FE}^{+++} + \text{HO}_2 + \text{OH}^-$ ; 6E4 (18)  
RE115:  $\text{H}^- + \text{H}_2\text{O} = \text{H}_2 + \text{OH}^-$ ; E6 (b)  
RE116:  $\text{O}_2^{--} + \text{H}_2\text{O} = \text{HO}_2^- + \text{OH}^-$ ; E6 (b)

#### Notes:

- (a) Calculated from refs. (18) and (19).
- (b) Balance reactions of no significance for the kinetics.

## 5. CHLORIDE REACTIONS

FILENAME=EB/CHLORIDE

This file contains reactions that are used for simulation of radiolysis of chloride in acid and neutral aqueous solution when combined with EB/WATER.

### References and notes

RE125: OH+CL[-]=CLOH[-]; 4.3E9  
RE126: OH+HCLO=CLO+H2O; 9E9  
RE127: OH+HCLO2=CLO2+H2O; 6.3E9  
RE128: E[-]+CL=CL[-]+H2O; E10  
RE129: E[-]+CL2[-]=2\*CL[-]+H2O; E10  
RE130: E[-]+CLOH[-]=CL[-]+OH[-]+H2O; E10 (a)  
RE131: E[-]+HCLO=CLOH[-]+H2O; 5.3E10  
RE132: E[-]+CL2=CL2[-]+H2O; E10 (a)  
RE133: E[-]+CL3[-]=CL2[-]+CL[-]+H2O; E10 (a)  
RE134: E[-]+HCLO2=CLO+OH[-]+H2O; 4.5E10  
RE135: E[-]+HCLO3=CLO2+OH[-]+H2O; 4E6  
RE136: H+CL=CL[-]+H[+]; E10 (a)  
RE137: H+CL2[-]=2\*CL[-]+H[+]; 8E9 (20)  
RE138: H+CLOH[-]=CL[-]+H2O; E10  
RE139: H+CL2=CL2[-]+H[+]; 7E9 (20)  
RE140: H+HCLO=CLOH[-]+H[+]; E10  
RE141: H+CL3[-]=CL2[-]+CL[-]+H[+]; E10  
RE142: H2O+CL2[-]=2\*CL[-]+O2+H[+]; 4E9  
RE143: H2O+CL2=CL2[-]+O2+H[+]; E9 (21)  
RE144: H2O+CL3[-]=CL2[-]+CL[-]+O2+H[+]; E9  
RE145: O2[-]+CL2[-]=2\*CL[-]+O2; 1.2E10 (20)  
RE146: O2[-]+HCLO=CLOH[-]+O2; 7.5E6 (22)  
RE147: H2O2+CL2[-]=2\*CL[-]+O2[-]+2\*H[+]; 1.4E5 (23)  
RE148: H2O2+CL2=H2O+CL2[-]+H[+]; 1.9E2 (24)  
RE149: H2O2+HCLO=CL[-]+O2+H2O+H[+]; 1.7E5 (25)  
RE150: OH[-]+CL2[-]=CLOH[-]+CL[-]; 7.3E6 (23)  
RE151: OH[-]+CL2=HCLO+CL[-]; 3.88E11 (b)  
RE152: H[+]+CLOH[-]=CL+H2O; 2.1E10 (26)  
RE153: H2O+CL2O2=HCLO+HCLO2; 2E2 (a)  
RE154: H2O+CL2O2=O2+HCLO+CL[-]+H[+]; E2 (a)

RE155:H2O+CL2O=2*HClO;E2	(a)
RE156:H2O+CL2O4=HClO2+HClO3;E2	(a)
RE157:H2O+CL2O4=2*O2+HClO+Cl[-]+H[+];E2	(a)
RE158:Cl[-]+Cl=Cl2[-];2.1E10	(26)
RE159:Cl[-]+ClOH[-]=Cl2[-]+OH[-];9E4	(27)
RE160:Cl[-]+HClO=Cl2+OH[-];10	(b)
RE161:Cl[-]+Cl2=Cl3[-];1E4	(c)
RE162:ClOH[-]=OH+Cl[-];6.1E9	(26)
RE163:Cl2[-]=Cl+Cl[-];1.1E5	(26)
RE164:Cl2[-]+Cl2[-]=Cl3[-]+Cl[-];7E9	
RE165:Cl3[-]=Cl2+Cl[-];5E4	(c)
RE166:ClO+ClO=Cl2O2;1.5E10	
RE167:ClO2+ClO2=Cl2O4;E2	(a)
RE168:Cl2O2+HClO2=HClO3+Cl2O;E2	(a)

Notes:

- (a) Reaction not known, arbitrary rate constant.
- (b) Based on eq.constant for  $Cl_2+H_2O=HClO+Cl[-]+H[+]$ ;  $K=3.88E-4$ , ref. (28).
- (c) Based on eq.constant for  $Cl_2+Cl[-]=Cl_3[-]$ ;  $K=0.18$ , ref. (28).

## 6. Fe-Cl REACTIONS

FILENAME=EB/FECL

This file contains reactions that are used for simulation of radiolysis of chloride + ferrous/ferric in aqueous solution when combined with EB/WATER, EB/FE, and EB/CHLORIDE.

### References and notes

RE170:CL+FE[++] = FE[+++]+CL[-];1.05E10	(29)
RE171:CLOH[-]+FE[++] = FE[+++]+CL[-]+OH[-];E8	
RE172:CL2[-]+FE[++] = FE[+++]+2*CL[-];1E7	
RE173:CL2+FE[++] = FE[+++]+CL2[-];80	(30)
RE174:HClO+FE[.] = FE[+++]+CLOH[-];3.6E3	(30)
RE175:CL3[-]+FE[++] = FE[+++]+CL2[-]+CL[-];2E5	(a)

### Notes:

(a) Estimated from ref. (31).

## 7. OZONE REACTIONS

FILENAME = EB/OZONE

This file contains reactions that are used for simulation of radiolysis of ozone in neutral and alkaline aqueous solution when combined with EB/WATER.

### References and notes

RE180:OH+O3=O2[-]+O2+H[+];1.1E8	(9)
RE181:E[-]+O3=O3[-]+H2O;3.6E10	(10)
RE182:H+O3=OH+O2;3.65E10	(10)
RE183:O[-]+O3=O2[-]+O2;E9	(a)
RE184:O2[-]+O3=O3[-]+O2;1.52E9	(10)
RE185:H02[-]+O3=O3[-]+O2[-]+H[+];3E6	(32)

### Notes:

(a) Estimated rate constant.

## 8. HIGH TEMPERATURE WATER REACTIONS

FILENAME=EB/H20TEMP

This file is used for simulation of radiolysis of water at high temperature (temperature constant or a function of time). After each reaction equation the activation energy  $E_a$  ( $\text{kcal}\cdot\text{mol}^{-1}$ ) and the frequency factor  $A$  are separated by a comma in writing. Where no reference is mentioned  $E_a$  is taken from Jenks estimated values (33,34).  $A$  is calculated from the rate constant at room temperature. The rate constants at  $T$  degree Kelvin is calculated from the Arrhenius equation:

$$k = A \cdot e^{-503.3 \cdot E_a / T}$$

### References and notes

RE1:OH+OH=H2O2;3,6.57E11  
RE2:OH+E[-]=OH[-]+H2O;3,3.28E12  
RE3:OH+H=H2O;3,4.1E12  
RE4:OH+H2=O2+H2O;3,1.3E12  
RE5:OH+O2[-]=O2+OH[-];3,1.64E12  
RE6:OH+H2O2=H2O+H2O;3,4,4.74E10 (8)  
RE7:OH+H2=H+H2O;4,6,8.44E10 (35)  
RE8:E[-]+E[-]=2\*OH[-]+H2;5,3,4.1E13  
RE9:E[-]+H=OH[-]+H2;3,3.28E12  
RE10:E[-]+H2O2=H2O2+OH[-];3,3.28E12  
RE11:E[-]+O2[-]=HO2[-]+OH[-];4,5,2.74E13  
RE12:E[-]+H2O2=OH+OH[-]+H2O;3,2.63E12  
RE13:E[-]+H[+]=H+H2O;3,3.61E12  
RE14:E[-]+H2O=H+OH[-]+H2O;3,3.28E3  
RE15:E[-]+O2=O2[-]+H2O;3,3.28E12  
RE16:H+H=H2;3,1.64E12  
RE17:H+H2O=H2O2;3,3.28E12  
RE18:H+O2[-]=HO2[-];3,3.28E12  
RE19:H+H2O2=OH+H2O;4,5,1.26E11  
RE20:H+OH[-]=E[-];3,3.28E9  
RE21:H+O2=HO2;3,3.28E12  
RE22:HO2+O2[-]=O2+HO2[-];4,5,1.79E11  
RE23:HO2=O2[-]+H[+];3,1.31E8



RE24:  $O_2[-] + H[+] = H_2O_2$ ; 3, 8.21E12

RE25:  $H_2O_2 + OH[-] = HO_2[-] + H_2O$ ; 4.5, 1.05E12

RE26:  $HO_2[-] + H_2O = H_2O_2 + OH[-]$ ; 3, 9.42E12

RE27:  $H_2O_2 = H_2O + O$ ; 17, 3.78E7

RE28:  $O + O = O_2$ ; 3, 1.64E12

RE29:  $H[+] + OH[-] = H_2O$ ; 3, 2.35E13

RE30:  $H_2O = H[+] + OH[-]$ ; 3, 4.27E-3

## 9. G-VALUES

### FILENAME=EB/GAMMA

This file contains G-values for low-LET electron and gamma irradiation of neutral water, ref. (36).

G(OH)=2.67  
G(E[-])=2.66  
G(H)=0.55  
G(H2)=0.45  
G(H2O2)=0.72  
G(H[+])=2.76  
G(OH[-])=0.1  
G(H2O)=-6.87

### FILENAME=EB/GAMMAPH046

This file contains G-values for low-LET electron and gamma irradiation of water pH=0.46, ref. (36).

G(OH)=2.89  
G(H)=3.62  
G(H2)=0.395  
G(H2O2)=0.76  
G(H[+])=0.1  
G(OH[-])=0.1  
G(H2O)=-4.51

**FILENAME=EB/GAMMAPH1**

This file contains G-values for low-LET electron and gamma irradiation of water pH=1, ref. (36).

G(OH)=2.83  
G(H)=3.55  
G(H2)=0.40  
G(H2O2)=0.76  
G(H[+])=0.1  
G(OH[-])=0.1  
G(H2O)=-4.45

**FILENAME=EB/GAMMAPH2**

This file contains G-values for low-LET electron and gamma irradiation of water pH=2, ref. (36).

G(OH)=2.74  
G(E[-])=2.80  
G(H)=0.55  
G(H2)=0.425  
G(H2O2)=0.73  
G(H[+])=2.90  
G(OH[-])=0.1  
G(H2O)=-7.10

**FILENAME=EB/GAMMAPH13**

This file contains G-values for low-LET electron and gamma irradiation of water pH=13, refs. (36,11).

G(OH)=3.0

G(E[-])=2.8

G(H)=0.55

G(H2)=0.425

G(HO2[-])=0.6

G(H[+])=3.90

G(OH[-])=0.5

G(H2O)=-7.50

**FILENAME=EB/GAMMAPH14**

This file contains G-values for low-LET electron and gamma irradiation of water pH=14, refs. (36,11).

G(OH)=3.3

G(E[-])=2.8

G(H)=0.55

G(H2)=0.425

G(HO2[-])=0.45

G(H[+])=3.75

G(OH[-])=0.5

G(H2O)=-7.50

**FILENAME=EB/N2OPH13**

This file contains G-values for low-LET electron and gamma irradiation of water pH=13, equilibrated with 4 MPa N<sub>2</sub>O, refs. (36,11).

G(E[-])=3.7  
G(H)=0.55  
G(OH)=3.4  
G(HO2[-])=0.6  
G(H2)=0.175  
G(H[+])=4.8  
G(OH[-])=0.5  
G(H2O)=-8.80

**FILENAME=EB/ALFA**

This file contains G-values for alfa irradiated neutral water. Based on refs. (37,38,39,40) and best fit to experiments, ref. (41).

G(OH)=.24  
G(E[-])=.06  
G(H)=0.21  
G(H2)=1.3  
G(H2O2)=0.985  
G(HO2)=0.22  
G(H[+])=0.06  
G(H2O)=-2.71

**FILENAME-EB/NEUTRON**

**This file contains G-values for neutron irradiated neutral water, ref. (37).**

**G(OH)=0.46**

**G(E[-])=0.37**

**G(H)=0.36**

**G(H2)=1.12**

**G(H2O2)=1.00**

**G(HO2)=0.17**

**G(H[+])=0.37**

**G(H2O)=-3.17**

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