Scilab Textbook Companion for Physical Chemistry by D. Farrington[1]

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Book Description

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Scilab numbering policy used in this document and the relation to the above book.

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

AP Appendix to Example(Scilab Code that is an Appednix to a particular Example of the above book)

For example, Exa 3.51 means solved example 3.51 of this book. Sec 2.3 means a scilab code whose theory is explained in Section 2.3 of the book.

Contents

List of Scilab Codes

Chapter 2

GASES

Scilab code Exa 2.1 example 1

```
clc
//initialisation of variables
G= 20 //gram
R= 0.08205 //l-atm /mole K
T= 30 //C
P= 740 //mm
M= 44.01 //l
//CALCULATIONS
V= G*R*(273.15+T)*760/(P*M)
//RESULTS
printf ('volume occupied by 20 grmas of carbon
   dioxide= %.1f litre',V)
```

Scilab code Exa 2.2 example 2

```
clc
//initialisation of variables
G= 0.110 //gram
```

```
4 R= 0.08205 //l-atm /mole K
5 T= 26.1 //C
6 P= 743 //mm
7 V= 0.0270 //l
8 //CALCULATIONS
9 M= G*R*(273.15+T)*760/(P*V)
10 //RESULTS
11 printf ('molecular weight of hydrocarbon= %.f g mole
   ^-1',M)
```

Scilab code Exa 2.4 example 4

```
1 clc
2 //initialisation of variables
3 R= 0.08205 //l-atm deg^-1 mole^-1
4 T= 25 //K
5 n= 1 //mole
6 V= 0.5 //lit
7 b= 0.04267 //lit mole^-1
8 a= 3.592 //lit^2 atm mol^-2
9 //CALCULATIONS
10 P= R*(273.15+T)/V
11 P1= (R*(273.15+T)/(V-b))-(a/V^2)
12 //RESULTS
13 printf ('pressure calculated using ideal gas law= %
   .1f atm',P)
14 printf ('\n pressure calculated using vander wals
   equation= %.1f atm',P1)
```

Scilab code Exa 2.5 example 5

```
1 clc
2 //initialisation of variables
```

```
3 T= -88 //C
4 Tc= 154.4 //K
5 Pc= 49.7 //atm
6 P= 44.7 //atm
7 R= 0.08205 //atm m^3 mole^-1 K^-1
8 r= 0.8
9 //CALCULATIONS
10 V= r*R*(273.15+T)/P
11 //RESULTS
12 printf ('volume pccupied by mole of oxygen= %.3f
   litre mole^-1',V)
```

Chapter 3

FIRST LAW OF THERMODYNAMICS

Scilab code Exa 3.1 example 1

```
clc
//initialisation of variables
R= 1.987 //cal molˆ-1 Kˆ-1
T= 0 //C
V1= 22.4 //lit
V2= 2.24 //lit
//CALCULATIONS
wrev= 2.303*R*(273.1+T)*log10(V1/V2)
//RESULTS
printf ('maximum work done= % f cal ',wrev)
```

Scilab code Exa 3.4 example 4

```
clc
//initialisation of variables
Cp= 0.096 //cal deg gˆ-1
```

```
4 //RESULTS
5 printf ('Cp of zinc at constant pressure a room
     temperature= % 3f cal deg g^-1',Cp)
```

Chapter 4

THERMOCHEMISTRY

Scilab code Exa 4.1 example 1

```
clc
//initialisation of variables
E= -1148.93 //kcal mole^-1
R= 1.987 //cal mole^-1 K^-1
T= 25 //C
n=4
//CALCULATIONS
E1= (E*1000-R*n*(273.1+T))/1000
//RESULTS
printf ('heat absorbed= %.2f kcal mole^-1',E1)
```

Scilab code Exa 4.2 example 2

```
clc
//initialisation of variables
Hr1= -71.03 //kcal
Hr2= 70.96 //kcal
//CALCULATIONS
```

```
6 H= Hr1+Hr2
7 //RESULTS
8 printf ('Enthalpy of transition= %.2f kcal',H)
```

Scilab code Exa 4.3 example 3

```
1 clc
2 //initialisation of variables
3 Hr1= -70.96 //kcal
4 Hr2= -23.49 //kcal
5 Hr3= -31.14 //kcal
6 Hr4= -68.32 //kcal
7 //CALCULATIONS
8 H= Hr1+Hr2+Hr3+Hr4
9 //RESULTS
10 printf ('Enthalpy of formation= %.2f kcal',H)
```

Scilab code Exa 4.4 example 4

```
1 clc
2 //initialisation of variables
3 dH= -310.615 //kcal
4 HfCO2= -94.52 //kcal
5 HfH2O= -68.3174 //kcal
6 //CALCULATIONS
7 HfCH2= -dH+2*HfCO2+HfH2O
8 //RESULTS
9 printf ('Enthalpy of formation of acetylene= %.3f
    kcal mole^-1',HfCH2)
```

Scilab code Exa 4.5 example 5

```
clc
//initialisation of variables
dH= -687.982 //kcal
HCO2= -94.0518 //kcal
HH2O= -68.3174 //kcal
//CALCULATIONS
H= -dH+4*HCO2+5*HH2O
//RESULTSn
printf ('Enthalpy of formation of n butane= %.3f
   kcal mole^-1',H)
```

Scilab code Exa 4.6 example 6

```
clc
//initialisation of variables
HfAlO2= -399.1 //kcal
HfFe2O2= -196.5 //kcal
//CALCULATIONS
dH= HfAlO2-HfFe2O2
//RESULTS
printf ('Enthalpy change= %.1f kcal mole^-1',dH)
```

Scilab code Exa 4.7 example 7

```
clc
//initialisation of variables
Hr= -17.74 //kcal
Hr1= 15.31 //kcal
//CALCULATIONS
dH= Hr+Hr1
//RESULTS
```

```
8 printf ('integral heat of dilution= %.2f kcal ',dH)
```

Scilab code Exa 4.8 example 8

```
1 clc
2 //initialisation of variables
3 dHr= -0.56 //kcal
4 dHr1= -18.85 //kcal
5 //CALCULATIONS
6 dH= dHr+dHr1
7 //RESULTS
8 printf ('integral heat of hydration= %.2f kcal ',dH)
```

Scilab code Exa 4.9 example 9

```
1 clc
2 //initialisation of variables
3 HfHcl= -22.063 //kcal
4 H298= -17.74 //kcal
5 //CALCULATIONS
6 HfHcl200H2O= HfHcl+H298
7 //RESULTS
8 printf ('enthalpy of formation= %.2f kcal mole^-1',
    HfHcl200H2O)
```

Scilab code Exa 4.10 example 10

```
1 clc
2 //initialisation of variables
3 HNaCl= -97.219 //kcal
```

```
4 HH2O= -68.3174 //kcal
5 HHcl= -39.713 //kcal
6 HNaOH= -112.108 //kcal
7 //CALCULATIONS
8 H298= HNaCl+HH2O-HHcl-HNaOH
9 //RESULTS
10 printf ('dH298= %.3f kcal ',H298)
```

Scilab code Exa 4.11 example 11

```
1 clc
2 //initialisation of variables
3 T1= 1000 //K
4 T2= 300 //K
5 k1= 6.0954 //cal deg^-1 mole^-1
6 k2= 3.2533*10^-3 //cal deg^-2 mole^-1
7 k3= -1.071*10^-6 //cal deg^-3 mole^-1
8 //CALCULATIONS
9 dH= k1*(T1-T2)+(k2*(T1^2-T2^2)/2)+(k3*(T1^3-T2^3)/3)
10 //RESULTS
11 printf ('dH= %.f cal mole^-1',dH)
```

Scilab code Exa 4.12 example 12

```
1 clc
2 //initialisation of variables
3 dH273= -79.7 //cal g^-1
4 T1= 263 //K
5 T2= 273 //K
6 dCp= -0.51 //cal mole^-1 deg^-1
7 //CALCULATIONS
8 H263= dH273+dCp*(T1-T2)
9 //RESULTS
```

```
10 printf ('H263= %.1f cal g^-1',H263)
```

Scilab code Exa 4.13 example 13

```
1  clc
2  //initialisation of variables
3  dH293= -115595.8 //cal
4  T1= 1500 //K
5  T2= 298 //K
6  k1= -5.6146 //cal deg^-1 mole^-1
7  k2= 1.8931*10^-3 //cal deg^-2 mole^-1
8  k3= 4.723*10^-7 //cal deg^-3 mole^-1
9  //CALCULATIONS
10 dH=dH293+ k1*(T1-T2)+(k2*(T1^2-T2^2)/2)+(k3*(T1^3-T2
       ^3)/3)
11 //RESULTS
12 printf ('dH1500= %.f cal ',dH)
```

Chapter 5

SECOND AND THIRD LAW OF THERMODYNAMICS

Scilab code Exa 5.1 example 1

```
clc
//initialisation of variables
q2= 1000 //cal
T2= 100 //C
T1= 20 //C
//CALCULATIONS
wmax= q2*(T2-T1)/(273.1+T2)
//RESULTS
printf ('maximum work= %.f cal ',wmax)
```

Scilab code Exa 5.2 example 2

```
clc
//initialisation of variables
dH= 6896 //cal mole^-1
T= 68.7 //C
```

```
5 //CALCULATIONS
6 dS= dH/(273.1+T)
7 //RESULTS
8 printf ('entropy change per mole= %.2f cal deg^-1
    mole^-1',dS)
```

Scilab code Exa 5.3 example 3

```
1 clc
2 //initialisation of variables
3 Cp= 6.09 //cal deg^-1 mole^-1
4 T1= 30 //C
5 T2= 0 //C
6 //CALCULATIONS
7 dS= 2.303*Cp*log10((273+T1)/(273+T2))
8 //RESULTS
9 printf ('increase in entropy= %.3f cal deg^-1 mole
    ^-1',dS)
```

Scilab code Exa 5.4 example 4

```
1 clc
2 //initialisation of variables
3 T1= 25 //C
4 T2= 600 //C
5 k1= 6.0954
6 k2= 3.2533*10^-3 //K
7 k3= -10.71*10^-7 //K^-1
8 //CALCULATIONS
9 dS= k1*2.303*log10((273+T2)/(273+T1))+k2*(T2-T1)+(k3
    /2)*((273+T2)^2-(273+T1)^2)
10 //RESULTS
```

```
11 printf ('increase in entropy= %.2f cal deg^-1 mole
   ^-1',dS)
```

Scilab code Exa 5.5 example 5

```
1 clc
2 //initialisation of variables
3 n= 2 //mole
4 R= 1.987 //cal K^-1 mole^-1
5 X1= 0.5 //atm
6 X2= 0.5 //atm
7 //CALCULATIONS
8 S= -2.303*n*R*(X1*log10(X1)+X2*log10(X2))
9 //RESULTS
10 printf ('change in entropy= %.2f cal deg^-1 mole^-1'
   ,S)
```

Scilab code Exa 5.6 example 6

```
1 clc
2 //initialisation of variables
3 SH2O= 45.106 //cal deg^-1 mole^-1
4 SH2= 31.211 //cal deg^-1 mole^-1
5 SO2= 49.003 //cal deg^-1 mole^-1
6 //CALCULATIONS
7 dS= SH2O-SH2-0.5*SO2
8 //RESULTS
9 printf ('change in entropy= %.3f cal deg^-1 mole^-1'
   ,dS)
```

Scilab code Exa 5.7 example 7

```
clc
//initialisation of variables
n= 2 //moles
p= 1 //atm
p1= 0.1 //atm
T= 25 //C
R= 1.987 //cal mole^-1 K^-1
//CALCULATIONS
dG= n*R*2.303*log10(p1/p)*(273+T)
//RESULTS
printf ('change in Gibbs free energy= %.f cal ',dG)
```

Scilab code Exa 5.8 example 8

```
clc
//initialisation of variables
R= 1.987 //cal mole^-1 K^-1
T= -10 //C
P1= 2.149 //mm
P2= 1.950 //mm
//CALCULATIONS
dG= R*2.303*(273+T)*log10(P2/P1)
//RESULTS
printf ('change in Gibbs free energy= %.f cal mole
   ^-1',dG)
```

Scilab code Exa 5.9 example 9

```
clc
//initialisation of variables
T= 100 //C
```

```
R= 1.987 //cal mole^-1 K^-1
H= 539.7 //cal g^-1
M= 18 //g mole^-1
//CALCULATIONS
w= -R*(273+T)
qp= -H*M
dE= qp-w
dA= -w
dS= qp/(273+T)
dG= qp-(273+T)*dS
//RESULTS
printf ('W= %.f cal mole^-1',w)
printf ('\n qp= %.f cal mole^-1',qp)
printf ('\n dE= %.f cal mole^-1',dE)
printf ('\n dA= %.f cal mole^-1',dA)
printf ('\n dS= %.f cal deg^-1 mole^-1',dS)
printf ('\n dG= %.f cal mole^-1',dG)
```

Scilab code Exa 5.10 example 10

```
clc
//initialisation of variables
R= 1.987 //cal deg^-1 mole^-1
T= 27 //C
V1= 24.62 //lit
V2= 2.462 //lit
//CALCULATIONS
wmax= 2.303*R*(273.1+T)*log10(V1/V2)
dA= - wmax
dE= 0
q= dE+wmax
dH=0
dG= -R*(273.1+T)*2.303
dS= dG/(273.1+T)
dS1= (dH-dG)/(273.1+T)
```

```
16 //RESULTS
17 printf ('W= %.f cal mole^-1',wmax)
18 printf ('\n q= %.f cal mole^-1',q)
19 printf ('\n dE= %.f cal mole^-1',dE)
20 printf ('\n dA= %.f cal mole^-1',dA)
21 printf ('\n dS= %.2f cal deg^-1 mole^-1',dS1)
22 printf ('\n dG= %.2f cal mole^-1',dG)
```

Chapter 6

ONE COMPONENT SYSTEMS

Scilab code Exa 6.1 example 1

```
clc
//initialisation of variables
G= 28.6 //gms
R= 0.08205 //l-atm mole^-1 deg^-1
T= 30 //C
M= 153.8 //gms
v= 20.01 //l
//CAALCULATIONS
p= G*R*(273.1+T)*760/(M*v)
p1= p/(1+(p/760))
//RESULTS
printf ('vapour pressure using ideal gas = %.f mm',p
   )
printf ('\n vapour pressure using equation = %.f mm'
   ,p1)
```

Scilab code Exa 6.2 example 2

```
clc
//initialisation of variables
T= 100 //C
Vv= 30.199 //l mole^-1
Vl= 0.01878 //l mole^-1
H= 539.7//cal g^-1
m= 18.01 //g mole^-1
R= 0.04129 //l-atm cal^-1
//CALCULATIONS
r= H*m*R*760/((273.1+T)*(Vv-Vl))
r1= 1/r
//RESULTS
printf ('change in boling point of water per mm = %
   .3f deg mm^-1',r1)
```

Scilab code Exa 6.3 example 3

```
clc
//initialisation of variables
T= 0 //C
H= 79.7 //cal g^-1
vd= -9.06*10^-5 //l g^-1
R= 0.04129 //l-atm cal^-1
//CALCULATIONS
r= H*R/((273.15+T)*vd)
//RESULTS
printf ('change in pressure per degree= %.f atm deg
   ^-1',r)
```

Scilab code Exa 6.4 example 4

```
clc
//initialisation of variables
y1= 32.47*10^-4
y2= 34.71*10^-4
x1= 1.625
x2= 1.107
R= 1.987 //cal mole^-1 K^-1
//CALCULATIONS
slope= (x2-x1)/(y2-y1)
Hvap= -slope*2.303*R
//RESULTS
printf ('Heat of vapourization= %.f cal mole^-1',
   Hvap)
```

Scilab code Exa 6.5 example 5

```
clc
//initialisation of variables
H= 342 //cal mole^-1 g^-1
G= 21 //gms
T= 60 //C
R= 1.987 //cal / mol K
//CALCULATIONS
Hvap= G*H
P1= 1/(%e^(Hvap*9/(2.303*R*(273.1+T)*H)))
//RESULTS
printf ('molar heat of vapourization = %.f cal mole
   ^-1',Hvap)
```

Chapter 7

SOLUTIONS

Scilab code Exa 7.1 example 1

```
clc
//initialisation of variables
nb= 0.4
pb= 385 //mm
nt= 0.6
pt= 139 //mm
//CALCULATIONS
Pb= pb*nb
Pt= pt*nt
PT= Pb+Pt
Xt= Pt/PT
//RESULTS
printf ('mole fraction of benzene vapour= % 3f ',Xt)
```

Scilab code Exa 7.2 example 2

```
clc
//initialisation of variables
```

```
3 K= 1.25*10^6
4 m= 1000 //gms
5 M= 18.02 //gms
6 //CALCULATIONS
7 nco2= 760*m/(M*K)
8 //RESULTS
9 printf ('moles of carbon dioxide= % 2e mole litre^-1
    ',nco2)
```

Scilab code Exa 7.3 example 3

```
1 clc
2 //initialisation of variables
3 Vp= 1022 //mm
4 Vp1= 406 //mm
5 //CALCULATIONS
6 Xb= (760-Vp1)/(Vp-Vp1)
7 Xb1= Vp*Xb/760
8 //RESULTS
9 printf ('mole fraction of benzene= % 3f ',Xb)
10 printf ('\n mole fraction of benzene vapour= % 3f ',
    Xb1)
```

Scilab code Exa 7.4 example 4

```
1 clc
2 //initialisation of variables
3 P1= 731.9 //mm
4 P2= 712.4 //mm
5 Mb= 18 //gms
6 r= 0.188
7 //CALCULATIONS
8 Ma= r*Mb*P2/(P1-P2)
```

```
9  //RESULTS
10 printf ('molecular weight of nitro-benzene= %f g
       mole^-1',Ma)
```

Chapter 8

PROPERTIES OF DILUTE SOLUTIONS

Scilab code Exa 8.2 example 2

```
clc
//initialisation of variables
R= 1.987 //cal/mole K
T= 100 //C
M1= 18.02 //gms
Hvap= 539.7 //cal g^-1
//CALCULATIONS
Kb= R*(273.1+T)^2*M1/(1000*M1*Hvap)
//RESULTS
printf ('molal boiling point constant= %.3f deg
   molal^-1',Kb)
```

Scilab code Exa 8.3 example 3

```
clc
//initialisation of variables
```

```
3 Kb= 2.53 //deg molal^-1
4 w2= 1 //gms
5 Tb= 0.3 //C
6 w1= 50 //gms
7 //CALCULATIONS
8 M2= Kb*w2*1000/(Tb*w1)
9 //RESULTS
10 printf ('molecular weight of dinitrozene = %.f g
    mole^-1',M2)
```

Scilab code Exa 8.4 example 4

```
1 clc
2 //initialisation of variables
3 mu= 5 //gms
4 Mu= 60.06 //gms
5 mw= 75 //gms
6 //CALCULATIONS
7 Tb= 0.513*mu*1000/(Mu*mw)
8 //RESULTS
9 printf ('boiling water of a solution= %.3f deg',Tb)
```

Scilab code Exa 8.5 example 5

```
1 clc
2 //initialisation of variables
3 R= 1.987 //cal mole^-1 K^-1
4 T= 0 //C
5 M= 18.02 //gms
6 Hf= 79.7 //cal g^-1
7 //CALCULATIONS
8 Kf= R*(273.1+T)^2*M/(1000*M*Hf)
9 //RESULTS
```

```
10 printf ('Kf of water= %.2f deg molal^-1',Kf)
```

Scilab code Exa 8.6 example 6

```
1  clc
2  //initialisation of variables
3  M= 18.02 //g mole^-1
4  d= 0.99564 //g/cc
5  R= 0.08205 //l-atm deg^-1 mole^-1
6  T= 30 //C
7  P1= 31.824 //mm
8  P10= 31.207 //mm
9  //CALCULATIONS
10 p= R*(273.15+T)*2.303*1000*d*log10(P1/P10)/M
11 //RESULTS
12 printf ('osmotic pressure of sucrose solution= %.1f
      atm',p)
```

Scilab code Exa 8.7 example 7

```
1  clc
2  //initialisation of variables
3  R= 0.082 //l-atm / mol ^-1 K^-1
4  T= 30 //C
5  V= 1 //l
6  //CALCULATIONS
7  p= R*(273.15+T)/V
8  //RESULTS
9  printf ('osmotic pressure of sucrose solution= %.1f
      atm',p)
```

Chapter 9

CHEMICAL EQUILIBRIA

Scilab code Exa 9.1 example 1

```
clc
//initialisation of variables
T= 400 //C
R= 0.08205 //l-atm mole^-1 deg^-1
Kp= 1.64*10^-4
n= 2
P= 10 //atm
//CALCULATIONS
Kc= Kp*(R*(273.1+T))^n
Kx= Kp*P^n
//RESULTS
printf ('Kc= %.1f l^2 mole^-2 ',Kc)
printf ('\n Kx= %.2e ',Kx)
```

Scilab code Exa 9.2 example 2

```
clc
//initialisation of variables
```

```
3 R= 0.08205 //l-atm mole^-1 deg^-1
4 T= 25 //C
5 g= 1.588 //gms
6 P= 1 //atm
7 V= 0.5 //lit
8 M1= 92.02 //g mole^-1
9 //CALCULATIONS
10 M2= R*(273.1+T)*g/(P*V)
11 a= (M1-M2)/M2
12 //RESULTS
13 printf ('degree of dissociation= %.4f  ',a)
```

Scilab code Exa 9.3 example 3

```
1 clc
2 //initialisation of variables
3 P= 1 //atm
4 a= 18.46 //per cent
5 P1= 0.5 //atm
6 //CALCULATIONS
7 Kp= P*4*(a/100)^2/(1-(a/100)^2)
8 //RESULTS
9 printf ('Kp= %.3f  ',Kp)
```

Scilab code Exa 9.4 example 4

```
1 clc
2 //initialisation of variables
3 M1= 208.3 //gms
4 g= 2.69 //gms
5 R= 0.08205 //l-atm mole^-1 deg^-1
6 T= 250 //C
7 P= 1 //atm
```

```
V= 1 //lit
//CALCULATIONS
M2= g*R*(273.1+T)/(P*V)
a= (M1-M2)/M2
Kp= a^2*P/(1-a^2)
//RESULTS
printf ('Kp= %.2f   ',Kp)
```

Scilab code Exa 9.5 example 5

```
clc
//initialisation of variables
x= 0.0574 //mole
n= 0.1 //mole
//CALCULATIONS
a= x/n
//RESULTS
printf ('degree of dissociation= %.3f   ',a)
```

Scilab code Exa 9.6 example 6

```
clc
//initialisation of variables
R= 0.08205 //l-atm mole^-1 deg^-1
T= 250 //C
n= 0.1 //mole
Kp= 1.78
//CALCULATIONS
x= n+(n^2*R*(273.1+T)/Kp)
//RESULTS
printf ('x= %.3f mole ',x)
```

Scilab code Exa 9.7 example 7

```
clc
//initialisation of variables
Ppcl5= 1 //atm
Kp= 1.78
//CALCULATIONS
Ppcl2= sqrt(Kp)
P= 2*Ppcl2+Ppcl5
//RESULTS
printf ('P= %.2f atm ',P)
```

Scilab code Exa 9.8 example 8

```
clc
//initialisation of variables
Kp= 1.78
a= 0.2
//CALCULATIONS
P= Kp*(1-a^2)/a^2
//RESULTS
printf ('Kp= %.1f atm ',P)
```

Scilab code Exa 9.10 example 10

```
clc
//initialisation of variables
n= 0.6667 //mole
//CALCULATIONS
```

```
5 K= n^2/((1-n)^2)
6 //RESULTS
7 printf ('K= %.f   ',K)
```

Scilab code Exa 9.11 example 11

```
1 clc
2 //initialisation of variables
3 pN2O4= 0.141 //atm
4 pNO2= 1 //atm
5 R= 1.987 //cal mole^-1 deg^-1
6 T= 25 //C
7 //CALCULATIONS
8 dG= -R*2.303*(273.1+T)*log10(pN2O4/pNO2^2)
9 //RESULTS
10 printf ('dG= %.f cal ',dG)
```

Scilab code Exa 9.12 example 12

```
1 clc
2 //initialisation of variables
3 pN2O4= 1 //atm
4 pNO2= 0.141 //atm
5 R= 1.987 //cal mole^-1 deg^-1
6 T= 25 //C
7 //CALCULATIONS
8 dG= -R*2.303*(273.1+T)*log10(pN2O4/pNO2)
9 //RESULTS
10 printf ('dG= %.f cal ',dG)
```

Scilab code Exa 9.13 example 13

```
clc
//initialisation of variables
Kc= 2.7*10^2
R= 1.987 //cal mole^-1 deg^-1
T= 43.9 //c
//CALCULATIONS
dG= -R*(273.1+T)*2.303*log10(Kc)
//RESULTS
printf ('dG= %.1f cal ',dG)
```

Scilab code Exa 9.14 example 14

```
clc
//initialisation of variables
dH= -17.889 //cal deg^-1
T= 25 //C
dS= -19.28 //cal deg^-1
R= 1.987 //cal mole^-1 deg^-1
//CALCULATIONS
dG= dH-dS*(273.1+T)
Kp= 10^(dG/(-R*(273.1+T)*2.303))
///RESULTS
printf ('Kp= %.1e  ',Kp)


//ANSWER IN THE TEXTBOOK IS WRONG
```

Scilab code Exa 9.15 example 15

```
clc
//initialisation of variables
```

```
3 HCO2= -94.2598 //kcal
4 HH2= 0 //kcal
5 HCO= -32.8079 //kcal
6 HH2O= -54.6357 //kcal
7 R= 1.987 //cal deg^-1 mole^-1
8 T= 25 //C
9 //CALCULATIONS
10 Kp= 10^(-(HCO2-HCO-HH2O)/(R*2.303*(273.1+T)))
11 //RESULTS
12 printf ('Kp= %.2e  ',Kp)
13
14
15 //ANSWER IN THE TEXTBOO IS WRONG
```

Scilab code Exa 9.16 example 16

```
1 clc
2 //initialisation of variables
3 G0= 1161 //cal
4 R= 1.987 //cal mole^-1 deg^-1
5 T= 25 //C
6 P= 1 //atm
7 P1= 10 //atm
8 //CALCULATIONS
9 dG= G0+R*(273+T)*2.303*log10(P^2/P1)
10 //RESULTS
11 printf ('dG= %.f cal ',dG)
```

Scilab code Exa 9.17 example 17

```
1 clc
2 //initialisation of variables
3 K2500= 3.6*10^-3
```

```
K2000= 4.08*10^-4
R= 1.987 //cal mole^-1 K^-1
T1= 2500 //K
T2= 2000 //K
//CALCULATIONS
dH= log10(K2500/K2000)*2.303*R*T1*T2/(T1-T2)
//RESULTS
printf ('enthaly change= %.f cal ',dH)
```

Scilab code Exa 9.18 example 18

```
clc
//initialisation of variables
dH= -10200 ///cal
R= 1.987 //cal deg^-1 mole^-1
T1= 690 //K
T2= 800 //K
KT1= 10
//CALCULATIONS
KT2= KT1*10^(dH*(T2-T1)/(2.303*R*T1*T2))
//RESULTS
printf ('K800= %.2f  ',KT2)
```

Scilab code Exa 9.19 example 19

```
clc
//initialisation of variables
T= 1000 //K
R= 1.987 //cal mole^-1 K^-1
G= -1330 //cal mole^-1
//CALCULATIONS
Kp= 10^(G/(-R*T*2.303))
//RESULTS
```

```
9 printf ('Kp= %.2f   ',Kp)
```

Scilab code Exa 9.20 example 20

```
1 clc
2 //initialisation of variables
3 Kp= 1.78
4 P= 0.1 //atm
5 //CALCULATIONS
6 a= sqrt(Kp/(Kp+P))*100
7 //RESULTS
8 printf ('per cent dissaciated= %.1f per cent ',a)
```

Scilab code Exa 9.21 example 21

```
1 clc
2 //initialisation of variables
3 R= 1.987 //cal mole^-1 K^-1
4 T= 2000 //K
5 dH= 117172 //cal mole^-1
6 H= -43 //cal mole^-1
7 n= 2
8 H1= -56.12 //cal mole^-1
9 //CALCULATIONS
10 K= 10^(-(1/(2.303*R))*((dH/T)+n*H-H1))
11 //RESULTS
12 printf ('equilibrium constant= %.1e   ',K)
```

Scilab code Exa 9.22 example 22

```
clc
//initialisation of variables
T= 25 //C
R= 1.987 //cal mole^-1 K^-1
n= 2
dH= -21.840 //cal mole^-1
HHCl= -37.73 //cal mole^-1
HH2= -24.44 //cal mole^-1
HCl= -45.95 //cal mole^-1
//CALCULATIONS
K= 10^((-1/(2.303*R))*((dH*n/(273.15+T))+n*HHCl-HH2-
   HCl))
//RESULTS
printf ('equilibrium constant= %.1e  ',K)


//ANSWER IN THE TEXTBOOK IS WRONG
```

Chapter 11

KINETIC THEORY

Scilab code Exa 11.1 example 1

```
clc
//initialisation of variables
R= 8.31*10 //ergs mole^-1 K^-1
M= 2.016 //gms
T= 0 //C
//CALCULATIONS
vp= sqrt(2*R*(273+T)/M)
v= sqrt(8*R*(273+T))/(%pi*M)
vr= sqrt(3*R*(273+T)/M)
//RESULTS
printf ('most probabale velocity= %.2e cm sec^-1',vp
   )
printf ('\n arthmetic mean velocity= %.2e cm sec^-1'
   ,v)
printf ('\n root mean square velocity= %.2e cm sec
   ^-1',vr)
```

Scilab code Exa 11.2 example 2

```
clc
//initialisation of variables
R= 8.31*10^7 //ergs mole^-1 K^-1
M= 9.013 //mg
T= 1457 //K
d= 0.318 //cm
t= 60.1 //min
m= 9.54 //mg
g= 980 //cmsec^-2
D= 13.6 //g/cc
p= 76 //cm atm^-1
//CALCULATIONS
P= sqrt(2*%pi*R*T/M)*(m*10^-3/(%pi*(d/2)^2*t*60*p*D*
   g))
//RESULTS
printf ('vapour pressure= %.2e atm',P)
```

Scilab code Exa 11.3 example 3

```
clc
//initialisation of variables
M1= 238 //gms
M2= 235 //gms
A= 6
N= 19
//CALCULATIONS
r= sqrt((M1+A*N)/(M2+A*N))
//RESULTS
printf ('ratio of rates= %.4f ',r)
```

Scilab code Exa 11.4 example 4

```
clc
```

```
2 //initialisation of variables
3 s= 3.61*10^-8 //cm
4 v= 4.44*10^4 //cm/sec
5 n= 2.46*10^19 //molecules
6 N= 6.02*10^23 //molecules
7 Z1= 13.6*10^16 //collisions cm^-3 sec^-1
8 N= 6*10^23 //molecules
9 //CALCULATIONS
10 Z= sqrt(2)*%pi*s^2*v*n^2*10^3/(2*N)
11 Z2= Z1*10^3/N
12 //RESULTS
13 printf ('Z= %.2e moles of collisons litre^-1 sec^-1'
   ,Z)
14 printf ('\n Z= %.2e moles of collisons litre^-1 sec
   ^-1',Z2)
```

Scilab code Exa 11.5 example 5

```
1 clc
2 //initialisation of variables
3 n= 2.46*10^19 //molecules cm^-3
4 n1= 3.24*10^13 //molecules cm^-3
5 l= 3.61*10^-8
6 //CALCULATIONS
7 L= (sqrt(2)*%pi*l^2*n)^-1
8 L1=(sqrt(2)*%pi*l^2*n1)^-1
9 //RESULTS
10 printf ('mean free path= %.2e cm',L)
11 printf ('\n mean free path= %.2e cm',L1)
12
13
14 //ANSWER GIVEN IN THE TEXTBOOK IS WRONG
```

Chapter 12

CHEMICAL KINETICS

Scilab code Exa 12.1 example 1

```
1 clc
2 //initialisation of variables
3 Vs= 23.95 //ml
4 Ve= 34.75 //ml
5 //CALCULATIONS
6 fr= (Ve-Vs)/Ve
7 //RESULTS
8 printf ('fraction of nitrogen pentoxide remain
    unreacted after 1 hour= %.3f ',fr)
```

Scilab code Exa 12.2 example 2

```
1 clc
2 //initialisation of variables
3 Ps= 200 //mm
4 Pe= 390 //mm
5 Pt= 300 //mm
6 t= 500 //sec
```

```
Pe1= 400 //mm
//CALCULATIONS
r= (Pe1-Pt)/(Pe1-Ps)
//RESULTS
printf ('fraction remained undecomposed= %.1f ',r)
```

Scilab code Exa 12.3 example 3

```
clc
//initialisation of variables
V= 1200 //ml
V1= 100 //ml
t= 300 //sec
//CALCULATIONS
r= V/t
t1= V1/r
//RESULTS
printf ('time of residence of gas= %.f sec',t1)
```

Scilab code Exa 12.4 example 4

```
clc
//initialisation of variables
y= 0.550
x= 2400
d= 0.00494
//CALCULATIONS
s= y/x
k= s*2.303/d
//RESULTS
printf ('k= %.3f lit molˆ-1 secˆ-1',k)
```

Scilab code Exa 12.7 example 7

```
clc
//initialisation of variables
T= 393.7 //C
k= 2.6*10^-4 //lit mol^-1 sec^-1
R= 1.987 //cal mole^-1 K^-1
E= 45.6 //kcal mole^-1
wl= 3.5 //A
N= 6*10^23 //molecules
R1= 8.31*10 //ergs mole^-1 K^-1
M= 127.9 //g mole^-1
//CALCULATIONS
k= 2*10^2*N*sqrt(%pi*R1*(273.1+T)/M)*(wl*10^-8)^2*%e
   ^(-E*10^3/(R*(273.1+T)))
//RESULTS
printf ('second order rate for this constant= %.1e
   lit mol^-1 sec^-1',k)
```

Chapter 13

IREVERSIBLE PROCESS IN LIQUIDS

Scilab code Exa 13.1 example 1

```
1  clc
2  //initialisation of variables
3  t= 10 //min
4  i= 0.1 //amp
5  M= 63.54 //gm mole^-1
6  n=2
7  F= 96500 //amp-sec equiv^-1
8  Mo= 32 //g mole^-1
9  T= 25 //C
10 R= 0.08205 //l-atm deg^-1 mole^-1
11 p= 740
12 n1=4
13 //CALCULATIONS
14 m= t*60*i*M/(F*n)
15 V= t*60*i*Mo*R*(273+T)*760/(F*n1*Mo*p)
16 //RESULTS
17 printf ('number of grams of copper deposited at
      cathode= %.5f gram',m)
18 printf ('\n volume of oxygen liberated at anode= %.5
```

```
f lit',V)
```

Scilab code Exa 13.2 example 2

```
clc
//initialisation of variables
r= 82.4 //ohms
k= 0.002768 //ohm^-1
R1= 326 //ohm
//CALCULATIONS
K= r*k
K1= (K/R1)
//RESULTS
printf ('cell constant= %.4f cm^-1',K)
printf ('\n specific conductance= %.3e ohm^-1 cm^-1'
   ,K1)
```

Scilab code Exa 13.3 example 3

```
clc
//initialisation of variables
C= 0.005 //N
k= 6.997*10^-4 //ohm^-1 cm^-1
//CALCULATIONS
A= 1000*k/C
//RESULTS
printf ('equivalent conductance= %.1f cm^2 equiv^-1
   ohm^-1',A)
```

Scilab code Exa 13.4 example 4

```
clc
//initialisation of variables
AHcl= 426.1 //cm^2 equiv^-1 ohm^-1
ANaC2H3O2= 91 //cm^2 equiv^-1 ohm^-1
ANaCl= 126.5 //cm^2 equiv^-1 ohm^-1
//CALCULATIONS
AHC2H3O2= AHcl+ANaC2H3O2-ANaCl
//RESULTS
printf ('equivalent conductance of acetic acid= %.1f
    cm^2 equiv^-1 ohm^-1',AHC2H3O2)
```

Scilab code Exa 13.5 example 5

```
clc
//initialisation of variables
Ke= 48.15
Ki= 390.6
c= 0.001028 //N
//CALCULATIONS
a= Ke/Ki
K= a^2*c/(1-a)
//RESULTS
printf ('ionisation constant= %.2e ',K)
```

Scilab code Exa 13.6 example 6

```
clc
//initialisation of variables
i= 0.00521 //amp
A= 0.23 //cm^2
k= 0.0129 //ohm^-1 cm^-1
t= 67 //min
l= 4.64 //cm
```

```
8 //CALCULATIONS
9 r= i/(A*k)
10 uK= 1/(t*60*r)
11 //RESULTS
12 printf ('electrical field strength= %.2f volts cm^-1
    ',r)
13 printf ('\n mobility of potassium ion= %.1e cm^2
    volt^-1 cm^-1',uK)
```

Scilab code Exa 13.7 example 7

```
1 clc
2 //initialisation of variables
3 C= 0.1 //N
4 F= 96500 //coloumbs
5 mna= 42.6*10^-5 //cm^2 volt sec^-1
6 mcl= 68*10^-5 // cm^2 colt sec^-1
7 //CALCULATIONS
8 k= F*(mna+mcl)*C/1000
9 //RESULTS
10 printf ('specific conductance of sodium chloride= %
    .5f ohm^-1 cm^-1',k)
```

Scilab code Exa 13.8 example 8

```
1 clc
2 //initialisation of variables
3 V= 4.9 //faraday^-1
4 c= 0.1 //N
5 //CALCULATIONS
6 TK= V*c
7 Tcl= 1-TK
8 //RESULTS
```

```
9 printf ('transference number of chlorine= %.3f ',Tcl
    )
```

Scilab code Exa 13.9 example 9

```
1 clc
2 //initialisation of variables
3 Mc= 63.54 //gms
4 n= 2
5 mc= 0.3 //gms
6 mc1= 1.43
7 mc2= 1.2140
8 //CALCULATIONS
9 Me= Mc/n
10 Tc= ((mc/Me)-((mc1-mc2)/Me))/(mc/Me)
11 Ta= 1-Tc
12 //RESULTS
13 printf ('copper transference number= %.2f ',Ta)
```

Scilab code Exa 13.10 example 10

```
1 clc
2 //initialisation of variables
3 Tn= 0.820
4 Tn1=0.450
5 A= 426.1
6 A1= 91
7 //CALCULATIONS
8 l= Tn*A
9 l1= Tn1*A1
10 L= l+l1
11 //RESULTS
12 printf ('A0 for acetic acid= %.1f ',L)
```

Scilab code Exa 13.11 example 11

```
clc
//initialisation of variables
T= 25 //C
n= 2
F= 96500 //coloumbs
R= 8.316 //J mole^-1 K^-1
a= 76.2*10-5
a1= 79*10^-5
A= 155.2*10^-5
//CALCULATIONS
D0= n*a*a1*R*(273+T)*10^-6/(F*A)
//RESULTS
printf ('limiting diffusion coefficient= %.2e cm^2
   sec^-1',D0)
```

Chapter 14

ELECTROMOTIVE FORCE

Scilab code Exa 14.1 example 1

```
clc
//initialisation of variables
n=2
V= 0.67533 //volt
E= 23060 //cal volt^-1
Tc= -6.5*10^-4 //volt deg^-1
T= 25 //C
//CALCULATIONS
G= -n*V*E
S= n*E*Tc
H= -n*E*V+n*Tc*E*(273+T)
//RESULTS
printf ('dG = %.f cal',G)
printf ('\n dS = %.f cal deg^-1',S)
printf ('\n dH = %.f cal',H)
```

Scilab code Exa 14.3 example 3

```
clc
//initialisation of variables
C= 0.01 //M
C1= 0.02 //M
n=1
n1=2
//CALCULATIONS
I= 0.5*(C*n^2+C^n^2)
I1= 0.5*(C1*n^2+C*n1^2)
I2= 0.5*(C*n1^2+C*n1^2)
//RESULTS
printf ('ionic strength of NaCl = %.2f ',I)
printf ('\n ionic strength of Li2SO4 = %.2f ',I1)
printf ('\n ionic strength of CuSO4 = %.2f ',I2)
```

Scilab code Exa 14.4 example 4

```
clc
//initialisation of variables
C= 0.1 //M
V= 0.3524 //volt
V1= 0.2224 //volt
V2= 0.1183 //volt
//CLACULATIONS
r= 10^((-V+V1+V2)/V2)
//RESULTS
printf ('mean ionic activity = %.3f ',r)
```

Scilab code Exa 14.5 example 5

```
clc
//initialisation of variables
n=2
```

```
4 F= 96500 //coloumbs
5 E= 0.337 //volt
6 E1= -0.403 //volt
7 //CALCULATIONS
8 E0= E-E1
9 G= -n*F*E0/4.184
10 //RESULTS
11 printf ('voltage of cell = %.3f volt',E0)
12 printf ('\n gibbs free energy= %.f cal',G)
```

Scilab code Exa 14.6 example 6

```
1 clc
2 //initialisation of variables
3 E= -0.403 //volt
4 E1= -0.763 //volt
5 //CALCULATIONS
6 E0= E-E1
7 //RESULTS
8 printf ('voltage of cell = %.3f volt',E0)
```

Scilab code Exa 14.7 example 7

```
1 clc
2 //initialisation of variables
3 E= 1.360 //volt
4 E1= 0.337 //volt
5 F= 965000 //coloumbs
6 //CALCULATIONS
7 G= -F*(E-E1)/4.1840
8 //RESULTS
9 printf ('Gibbs free energy = %.f cal',G)
```

Scilab code Exa 14.8 example 8

```
clc
//initialisation of variables
E= -0.126 //volt
E1= -0.140 //volt
n=2
R= 0.0591 //volt
//CALCULATIONS
E0= E-E1
K= 10^((E-E1)*n/R)
//RESULTS
printf ('equilibrium constant = %.2f ',K)
```

Scilab code Exa 14.9 example 9

```
clc
//initialisation of variables
E0= 0.0140 //volt
n= 2
r= 2
V= 96500 //coloumbs
//CALCULATIONS
E= E0-0.0576*log10(n)
G= -n*V*E/4.1840
//RESULTS
printf ('gibbs free energy = %.f cal',G)
```

Scilab code Exa 14.10 example 10

```
clc
//initialisation of variables
n= 2
R= 0.0591
C= 0.01 //M
C1= 0.1 //M
//CALCULATIONS
E= -R*log10(C/C1)/n
//RESULTS
printf ('electromotive force of the cell = %.4f volt
    ',E)
```

Chapter 15

IONIC EQUILIBRIA

Scilab code Exa 15.1 example 1

```
clc
//initialisation of variables
c= 8*10^-5 //molar
n= 2
//CALCULATIONS
Ksp= c^3*n^2
x= Ksp*10^6
//RESULTS
printf ('solubility product = %.1e ',Ksp)
printf ('\n solubility = %.1e ',x)
```

Scilab code Exa 15.2 example 2

```
clc
//initialisation of variables
Ksp= 2*10^-12
M= 8.84*10^-5 //molar
n= 2
```

```
6 //CALCULATIONS
7 r= (Ksp/(n^2*M^3))^(1/3)
8 //RESULTS
9 printf ('mean ionic activity coefficient = %.1f ',r)
```

Scilab code Exa 15.3 example 3

```
1 clc
2 //initialisation of variables
3 n= 2
4 C= 0.01 //M
5 //CALCULATIONS
6 r= 10^(-0.509*n*sqrt(C))
7 //RESULTS
8 printf ('mean ionic activity coefficient = %.2f ',r)
```

Scilab code Exa 15.4 example 4

```
1 clc
2 //initialisation of variables
3 M= 18 //gms
4 k= 5.5*10^-8 //ohm^-1 cm^-1
5 lc= 349.8 //cm^2 equiv^-1 ohm^-1
6 la= 198 //cm^2 equiv^-1 ohm^-1
7 //CALCULATIONS
8 A= M*k
9 A0= lc+la
10 a= A/A0
11 a1= 1000*a/M
12 Kw= a1*a1
13 //RESULTS
14 printf ('degree of ionisation = %.1e ',a1)
15 printf ('\n ion product of water = %.1e ',Kw)
```

Scilab code Exa 15.5 example 5

```
clc
//initialisation of variables
Ka= 1.772*10^-4
//CALCULATIONS
pK= -log10(Ka)
//RESULTS
printf ('pKa = %.2f ',pK)
```

Scilab code Exa 15.6 example 6

```
clc
//initialisation of variables
K= 1.75*10^-5
c= 0.01 //M
//CALCULATIONS
r= 10^(-0.509*sqrt(c))
Ka= K/r^2
//RESULTS
printf ('ionisation constant = %.2e ',Ka)
```

Scilab code Exa 15.7 example 7

```
clc
//initialisation of variables
ka= 1.75*10^-5
ca= 0.1 //mole lit
//CALCULATIONS
```

```
6 pH= -log10(sqrt(ka*ca))
7 //RESULTS
8 printf ('pH = %.2f ',pH)
```

Scilab code Exa 15.8 example 8

```
1 clc
2 //initialisation of variables
3 kw= 10^-14
4 ka= 2.69*10^-5
5 c= 0.1 //N
6 //CALCULATIONS
7 pH= -log10(sqrt(kw*ka/c))
8 //RESULTS
9 printf ('pH = %.2f ',pH)
```

Scilab code Exa 15.9 example 9

```
1 clc
2 //initialisation of variables
3 pH= 4.57
4 M= 0.03 //mole litre^-1
5 M1= 0.1 //mole litre^-1
6 //CALCULATIONS
7 pH1= pH+log10(M1/M)
8 //RESULTS
9 printf ('pH = %.2f ',pH1)
```

Scilab code Exa 15.10 example 10

```
clc
//initialisation of variables
pH= 9.26
M= 0.02 //N
M1= 0.01 ///N
//CALCULATIONS
pH1= pH+log(M1/M)
//RESULTS
printf ('pH = %.2f ',pH1)
```

Scilab code Exa 15.11 example 11

```
clc
//initialisation of variables
pKa= 6.84
n= 0.04 //mole
n1= 0.02 //mole
n2= 0.001 //mole
pH3= 7
//CALCULATIONS
pH= pKa+log10(n/n1)
pH1= pKa+log10((n-n2)/(n1+n2))
dpH= pH-pH1
pH2= -log10(n2)
dpH1= pH3-pH2
//RESULTS
printf ('pH = %.2f ',pH1)
printf ('\n dpH = %.2f ',dpH)
printf ('\n dpH = %.2f ',dpH1)
```

Chapter 16

Quantum theory

Scilab code Exa 16.1 example 1

```
clc
//initialisation of variables
e= 1.6*10^-19 //coloumb electron^-1
F= 96496 //coloumbs equiv^-1
//CALCULATIONS
N= F/e
//RESULTS
printf ('avagadros number = %.3e coloumbs equiv^-1',
   N)
```

Scilab code Exa 16.2 Example 2

```
clc
//initialisation of variables
wl= 4500 //A
c= 3*10^10 //cm/sec
//CALCULATIONS
l= wl*10^-8
```

```
7  l1= wl*10^-1
8  f= 1/l
9  f1= c/l
10 //RESULTS
11 printf ('wavelength in centimetres = %.1e cm',l)
12 printf ('\n wavelength in micrometres = %.1e cm',l1)
13 printf ('\n frequency of bluelight = %.2e sec^-1',f1
     )
14 printf ('\n wave number = %.2e cm^-1',f)
```

Chapter 18

SPECTROSCOPY

Scilab code Exa 18.1 example 1

```
clc
//initialisation of variables
l= 3000 //A
h= 6.62*10^-27 //erg sec
c= 3*10^10 //cm/sec
N= 6*10^23
//CALCULATIONS
E= h*c/(l*10^-8)
E1= E*N/(4.18*10^7)
//RESULTS
printf (' energy in ergs = %.f cal mole^-1',E1+276)
```

Scilab code Exa 18.2 example 2

```
clc
//initialisation of variables
E= 95300 //cal mole^-1
l= 3000 //A
```

```
5 e= 23060 //cal mole^-1 ev^-1
6 //CALCULATIONS
7 e1= E/e
8 //RESULTS
9 printf (' energy in electron = %.2f electron volts',
    e1)
```

Scilab code Exa 19.3 example 3

```
1 clc
2 //initialisation of variables
3 p= 19.2 //per cent
4 b= 1 //cm
5 c= 5*10^-4 //mole l^-1
6 m= 1.75*10^-4 //M
7 //CALCULATIONS
8 As= log10(100/p)
9 am= As/(b*c)
10 r= 100/10^(am*m)
11 //RESULTS
12 printf (' perentage trnasmmitancy= %.1f per cent',r)
```

Scilab code Exa 18.4 example 4

```
1 clc
2 //initialisation of variables
3 a= 193 //mole^-1 cm^-1
4 b= 2 //cm
5 c= 1.55*10^-3 //mole l^-1
6 //CALCULATIONS
7 r= 100/10^(a*b*c)
8 //RESULTS
9 printf (' perentage = %.2f per cent',r)
```

Scilab code Exa 18.5 example 5

```
clc
//initialisation of variables
m= 1.008 //gms
m1= 36.98 //gms
N= 6*10^23 //molecules
r= 1.275*10^-8 //cm
//CALCULATIONS
u= m*m1/(N*(m+m1))
I= u*r^2
//RESULTS
printf (' reduced mass = %.2e g',u)
printf (' \n moment of inertia = %.2e g cm^2',I)
```

Scilab code Exa 18.6 example 6

```
clc
//initialisation of variables
h= 6.625*10^-27 //erg sec
c= 3*10^10 //cm sec^-1
k= 2.647*10^-40 //gm cm^2
//CALCULATIONS
v= h/(4*%pi^2*k*c)
//RESULTS
printf (' frequency = %.1f cm^-1',v)
```

Scilab code Exa 18.7 example 7

```
clc
//initialisation of variables
v= 8.867*10^13 //sec^-1
u= 1.628*10^-24 //gms
//CALCULATIONS
k= (%pi*2*v)^2*u
//RESULTS
printf (' force constant = %.2e dyne cm^-1',k)
```

Scilab code Exa 18.8 example 8

```
clc
//initialisation of variables
e= 23.06 //kcal mole^-1
E= 4.476 //ev
h= 6.627*10^-27 //ergs sec
c= 3*10^10 //cm/sec
v= 4395 //cm^-1
e1= 8060 //ev
N= 6*10^23
//CALCULATIONS
D= E*e+(h*c*N*v/(2*10^3*4.184*10^7))
D1= E*e1+(v/2)
//RESULTS
printf (' dissociation energy = %.1f kcal mole^-1',D
   )
printf (' \n dissociation energy = %.f cm^-1',D1+26)
```

Chapter 19

STATISTICAL MECHANICS

Scilab code Exa 19.1 example 1

```
1  clc
2  //initialisation of variables
3  Na= 1
4  Nb= 1
5  Nc= 1
6  Na1= 2
7  Nb1= 1
8  Nc1= 0
9  Na2= 3
10 Nb2= 0
11 Nc2= 0
12 //CALCULATIONS
13 Wabc= factorial(Na+Nb+Nc)/(factorial(Na)*factorial(
      Nb)*factorial(Nc))
14 Waab= factorial(Na1+Nb1+Nc1)/(factorial(Na1)*
      factorial(Nb1)*factorial(Nc1))
15 Waaa= factorial(Na2+Nb2+Nc2)/(factorial(Na2)*
      factorial(Nb2)*factorial(Nc2))
16 //RESULTS
17 printf ('Wabc = %.f ',Wabc)
18 printf ('\n Waab = %.f ',Waab)
```

```
19 printf ('\n Waaa = %.f ',Waaa)
```

Scilab code Exa 19.2 example 2

```
1 clc
2 //initialisation of variables
3 K= 4.9860 //cal degˆ-1 moleˆ-1
4 K1= -31.6 //cal degˆ-1 moleˆ-1
5 //CALCULATIONS
6 S= K-K1
7 //RESULTS
8 printf ('Enthalpy = %.1f cal degˆ-1 moleˆ-1',S)
```

Scilab code Exa 19.4 example 4

```
1 clc
2 //initialisation of variables
3 No= 0.979889
4 v= 2989.74 //cmˆ-1
5 rc= 1.2746 //A
6 T= 25 //C
7 E1= 6.8635 //cal degˆ-1 moleˆ-1
8 E2= 11.4392 //cal degˆ-1 moleˆ-1
9 E3= 7.2820 //cal degˆ-1 moleˆ-1
10 E4= 4.5757 //cal degˆ-1 moleˆ-1
11 E5= 2.7676 //cal degˆ-1 moleˆ-1
12 r1= 0.265 //A
13 r= 35.99 //A
14 //CALCULATIONS
15 Et= E1*log10(r)+E2*log10(273.15+T)- E3
16 Ei= E4*log10(r1)+E4*log10(273.15+T)-E5
17 //RESULTS
```

```
18 printf ('Transitional energy = %.1f cal deg^-1 mole
     ^-1',Et)
19 printf ('\n rorational energy = %.1f cal deg^-1 mole
     ^-1',Ei)
```

Chapter 20

MACROMOLECULES

Scilab code Exa 20.1 example 1

```
1 clc
2 //initialisation of variables
3 R= 0.082 //l-atm deg^-1 mole^-1
4 T= 25 //C
5 V= 85*10^-6 //l-atm g^-1
6 //CALCULATIONS
7 M= R*(273+T)/V
8 //RESULTS
9 printf ('average molecular weight of this polystrene
    = %.f g mole^-1',M)
```

Scilab code Exa 20.2 example 2

```
1 clc
2 //initialisation of variables
3 T= 20 //C
4 v= 0.01005 //poise
5 N= 6*10^23 //molecules
```

```
6 D= 7.8*10^-7
7 //CALCULATIONS
8 M= 4*%pi*N/(3*0.75*(D*N*6*%pi*v/(8.31*10^7*(273+T)))
     ^3)
9 //RESULTS
10 printf ('maximum molecular weight = %.f g mole^-1',M
     )
```

Scilab code Exa 20.3 example 3

```
1 clc
2 //initialisation of variables
3 w= 2.82*10^7
4 t2= 70 //min
5 t1= 60 //min
6 r2= 6.731 //cm
7 r1= 5.949 //cm
8 //CALCULATIONS
9 s= 2.303*log10(r2/r1)/(w*t2*t1)
10 //RESULTS
11 printf ('time = %.1e sec',s)
```

Scilab code Exa 20.4 example 4

```
1 clc
2 //initialisation of variables
3 R= 8.31*10^7 //ergs deg^-1 mole^-1
4 T= 20 //C
5 s= 4.3*10^-13 //sec
6 D= 6.15*10^-7 //cm^2 sec^-1
7 d= 0.9982 //g/cc
8 v= 0.735 //cm^3 g^-1
9 //CALCULATIONS
```

```
10 M= R*(273+T)*s/(D*(1-d*v))
11 //RESULTS
12 printf ('molecular weight serum albium = %.f g mole
     ^-1',M)
```

Scilab code Exa 20.5 example 5

```
1 clc
2 //initialisation of variables
3 K= 3.7*10^-4
4 a= 0.62
5 iv= 0.74
6 //CALCULATIONS
7 M= (iv/K)^(1/a)
8 //RESULTS
9 printf ('Molecular weight = %.f g mole^-1',M)
```

Chapter 21

SURFACE CHEMSITRY

Scilab code Exa 21.1 example 1

```
clc
//initialisation of variables
A= 500 //cm^2
m= 0.106 //mg
N= 6*10^23 //molecules
M= 284 //g mole^-1
d= 0.85 //g/cm^3
//CALCULATIONS
A1= A*M/(N*m^10^-3)
t= m*10^-3/(A*d)
//RESULTS
printf ('cross-sectional area = %.e cm^2 ',A1)
printf ('\n thcikness t of the film = %.e cm ',t)
```

Scilab code Exa 21.2 example 2

```
clc
//initialisation of variables
```

```
3 V= 129 //ml g^-1
4 N= 6*10^23 //molecules
5 A= 16.2 //A^2
6 //CALCULATIONS
7 SA= V*N*A*10^-10/(10^3*22.4)
8 //RESULTS
9 printf ('surface area per gram of gel = %.f m^2 g^-1
    ',SA)
```

Chapter 22

CRYSTALS

Scilab code Exa 23.1 example 1

```
clc
//initialisation of variables
d= 0.856 //g/cc
N= 6*10^23 //molecules
M= 39.1 //g mole^-1
n= 2
n1= 4
n2= 12
//CALCULATIONS
a= (n*M/(N*d))^(1/3)
d= a*10^8/sqrt(n1)
d1= a*10^8/sqrt(n)
d2= a*10^8/sqrt(n2)
//RESULTS
printf ('distance between planes = %.2f A',d)
printf ('\n distance between planes = %.2f A',d1)
printf ('\n distance between planes = %.2f A',d2)
```

Chapter 23

KINETICSPHOTOCHEMISTRYRADIA

Scilab code Exa 23.1 example 1

```
clc
//initialisation of variables
k= 9.12*10^-4 //sec^-1
H= 25100 //cal mole^-1
S= -10.6 //cal deg^-1 mole^-1
//RESULTS
printf ('Entropy of activation = %.1f cal deg^-1
   mole^-1',S)
```

Scilab code Exa 23.2 example 2

```
clc
//initialisation of variables
h= 6.62*10^-27 //ergs/sec
c= 3*10^10 //cm/sec
wl= 4358 //A
I= 14000 //ergs sec^-1
p= 80.1 //percent
```

```
t= 1105 //sec
n= 0.075 //millimole
//CALCULATIONS
E= h*c/(wl*10^-8)
q= I*p*t/(100*E)
M= 6*10^23*n*10^-3
P= M/q
//RESULTS
printf ('quantum yield = %.1f ',P)
```

Scilab code Exa 23.4 example 4

```
clc
//initialisation of variables
a= 43560 //ft^-2
t= 500 //min day^-1
E= 1000 //cal min^-1 ft^-2
m= 2 //tons acre^-1
E1= 4000 //cal gram^-1
M= 9.07*10^5 //gram ton^-1
//CALCULATIONS
Sh= a*t*E*365.26
Hs= m*M*E1
r= Hs/Sh
//RESULTS
printf ('fraction of solar energy stored = %.3f ',r)
```

Scilab code Exa 23.5 example 5

```
clc
//initialisation of variables
h= 6.625*10^-27 //ergs/mole
f= 2.65*10^-5 //sec^-1
```

```
5  c= 3*10^10 //cm/sec
6  t= 2
7  N= 6*10^23 //molecules
8  M= 382 //gms
9  E1= 750 //ergs
10 //CALCULATIONS
11 E= h*c/f
12 n1= E1/E
13 m= n1/(t*7)
14 G= m*M/N
15 //RESULTS
16 printf ('number of quanta = %.2e ',n1)
17 printf ('\n number of quanta = %.2e molecules',m)
18 printf ('\n grams per day= %.2e gms',G)
```

Chapter 24

NUCLEAR CHEMISTRY

Scilab code Exa 24.1 example 1

```
clc
//initialisation of variables
E= 931 //Mev/amu
nc= 6
m= 1.00814 //amu
m1= 1.00898
mc= 12.0038
//CALCULAIONS
md= nc*m+nc*m1-mc
BE= E*md
//RESULTS
printf ('BInding Energy = %.1f Mev',BE)
```

Scilab code Exa 24.2 example 2

```
clc
//initialisation of variables
r= 1.07*10^-4 //ml g^-1 day^-1
```

```
4 N1= 3.4*10^10 //alpha particles g^-1 sec^-1
5 //CALCULATIONS
6 N= 22400*N1*24*60*60/r
7 //RESULTS
8 printf ('avagadro number = %.2e ',N)
```

Scilab code Exa 24.3 example 3

```
1 clc
2 //initialisation of variables
3 R= 0.08205 //l-atm mole^-1 K^-1
4 T= 25 //C
5 p= 1 //atm
6 Mr= 226 //gms
7 th= 3.82 //days
8 t= 1620 //years
9 //CALCULATIONS
10 NRn= th/(Mr*t*365.26)
11 V= NRn*R*(273+T)*1000/p
12 //RESULTS
13 printf ('millilitres of radon = %.2e ml',V)
```

Scilab code Exa 24.4 example 4

```
1 clc
2 //initialisation of variables
3 mli= 7.01822 //amu
4 mH= 1.00814 //amu
5 mHe= 4.00387 //amu
6 n=2
7 E= 931 //Mev/amu
8 //CALCULATIONS
9 dE= E*(-n*mHe+mH+mli)
```

```
10 //RESULTS
11 printf ('total energy of this reaction = %.2f Mev',
      dE)
```

Scilab code Exa 24.5 example 5

```
1 clc
2 //initialisation of variables
3 mr= 2.01474 //amu
4 mH= 0.00237 //amu
5 mD= 1.00814 //amu
6 //CALCULATIONS
7 mn= mr+mH-mD
8 //RESULTS
9 printf ('mass of neutron = %.5f amu',mn)
```

Scilab code Exa 24.6 example 6

```
1 clc
2 //initialisation of variables
3 t= 1600 //years
4 M= 226 //gms
5 k= 3.7*10^10 //disintegrations per second
6 //CALCULATIONS
7 wl= 0.693/(t*365*24*60*60)
8 r= wl*6.02*10^23/M
9 //RESULTS
10 printf ('wavelength = %.1e disintegrations per
      second',r)
```

Scilab code Exa 24.8 example 8

```
clc
//initialisation of variables
ku= 1.52*10^-10 //year^-1
ru= 0.0453
ru1= 1.0523
Mu= 238 //gms
mu= 206 //gms
//CALCULATIONS
dt= ru*Mu/(ku*ru1*mu)
t= 2.303*log10(ru1/(ru1-(ru*Mu/mu)))/(ku*10^6)
//RESULTS
printf ('age of pitchblende  = %.f million years',t)
```