Scilab Textbook Companion for Physical Chemistry by G. H. Duffey[1]

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Book Description

Title: Physical Chemistry

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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 1

Matter and its atomic nature

Scilab code Exa 1.1 Example 1

```
clc
//Initialization of variables
l=0.71 *10^-8 //cm
n=200 //lines/cm
v=0.00145 //radian
//calculations
d=1/n
phi2=2*l/d +v^2
phi=sqrt(phi2)
//results
printf('Angle required = %.2e radian',phi)
```

Scilab code Exa 1.2 Example 2

```
clc
//Initialization of variables
angle=37.25 //degrees
l=1.539 //A
```

```
5 n=1 //order
6 //calculations
7 d=n*l/(2*sind(angle))
8 //results
9 printf("Interplanar distance = %.3f A",d)
```

Scilab code Exa 1.5 Example 5

```
1 clc
2 //Initialization of variables
3 r1=sqrt(3)
4 r2=1
5 //calculations
6 ratio=r1-r2
7 //results
8 printf('Ratio of radii = %.3f',ratio)
```

Scilab code Exa 1.6 Example 6

```
1 clc
2 //Initialization of variables
3 d=2.64 //g/cc
4 l=4.016*10^-8 //cm
5 n=4
6 M=25.94 //g/mol
7 //calculations
8 m=d*l^3 /n
9 N0=M/m
10 //results
11 printf("Avagadro number = %.3e molecule/mol",N0)
```

Scilab code Exa 1.10 Example 10

```
clc
//Initialization of variables
A=[-1 -1 -1 ]
B=[1 1 -1]
//calculations
Ad=sqrt(1+1+1)
Bd=sqrt(1+1+1)
dot=A.*B /(Ad*Bd)
theta=acosd(dot)
//results
printf("Angle = %.2f degrees",theta(1,1))
```

Chapter 2

Particles Atomic and subatomic

Scilab code Exa 2.2 Example 2

```
1 clc
2 //Initialization of variables
3 m1=1.008142
4 m2=1.008982
5 //calculations
6 dm=m1-m2
7 dt=abs(dm) *931
8 //results
9 printf("Increase in kinetic energy = %.3f Mev",dt)
```

Scilab code Exa 2.3 Example 3

```
1 clc
2 //Initialization of variables
3 d=8.642 //g/cc
4 M=112.41 //g/mol
5 ratio=0.01/100
6 nb=2400
```

```
7 //calculations
8 n=d*6.02*10^23 /M
9 sigma=nb*10^-24
10 x=-2.303*log10(ratio) /(sigma*n)
11 //results
12 printf("Thickness = %.3f cm",x)
```

Scilab code Exa 2.4 Example 4

```
1 clc
2 //Initialization of variables
3 M1=4
4 M2=14
5 E=-1.2 //Mev
6 //calculations
7 R1=1.5*10^-13 *(M1)^(1/3)
8 R2=1.5*10^-13 *(M2)^(1/3)
9 V1=2*7*(4.8*10^-10)^2 /(R1+R2)
10 V2=V1/(1.6*10^-6)
11 x=(M1+M2)*V2/M2
12 //results
13 printf("Threshold = %.1f Mev",x)
```

Scilab code Exa 2.6 Example 6

```
1 clc
2 //Initialization of variables
3 t=1622 //years
4 per=1 //percent
5 //calculations
6 Nratio=1-per/100
7 x=t*log10(Nratio) / log10(0.5)
8 //results
```

```
9 printf("Time taken = %.1f years",x)
```

Chapter 3

Waves and Quanta

Scilab code Exa 3.9 Example 9

```
1 clc
2 //initialization of variables
3 atoms=5
4 //calculations
5 f=3*atoms
6 fvib=f-3-3
7 //results
8 printf("Vibrational degrees of freedom = %d",fvib)
```

Chapter 4

Molecular energy levels

Scilab code Exa 4.1 Example 1

```
clc
//initialization of variables
B=10.34 //cm^-1
c=2.998*10^10 //cm/s
h=6.625*10^-27 //erg sec
//calculations
I=h/(8*%pi^2 *B*c)
//results
printf("Moment of inertia = %.2e g cm^2",I)
```

Scilab code Exa 4.2 Example 2

```
clc
//Initialization of variables
ma=1.0080
mb=35.457
Na=6.0232*10^23
I=2.707*10^-40 //g cm^2
```

```
7 //calculations
8 mu1=ma*mb/(ma+mb)
9 mu2=mu1/Na
10 r=sqrt(I/mu2)
11 //results
12 printf("Bond length = %.2e cm",r)
```

Scilab code Exa 4.3 Example 3

```
1 clc
2 //Initialization of variables
3 c=2.998*10^10 //cm/s
4 wave=2990 //cm^-1
5 mu=1.627*10^-24 //g
6 //calculations
7 k=mu*(2*%pi*c*wave)^2
8 //results
9 printf("Force constant = %.2e dynes/cm",k)
```

Scilab code Exa 4.4 Example 4

```
1 clc
2 //initialization of variables
3 l1=2886 //cm^-1
4 l2=5668 //cm^-1
5 //calculations
6 wave=2*l1-l2
7 wave2= wave+l1
8 x=wave/(2*wave2)
9 //results
10 printf("anharmonicity constant = %.4f ",x)
```

Chapter 6

Valence electrons in molecules

Scilab code Exa 6.1 Example 1

```
1 clc
2 //initialization of variables
3 a2=1/8
4 //calculations
5 b2=1-a2
6 a1=sqrt(a2)
7 b1=sqrt(b2)
8 //results
9 printf(" Wave function is %.2f phi1 +%.2f phi2",a1,
    b1)
```

Scilab code Exa 6.3 Example 3

```
1 clc
2 //initialization of variables
3 sinu=2/sqrt(3)
4 cosu=sqrt(2/3)
5 //calculations
```

```
6 tanu=sinu/cosu
7 u=atand(sinu/cosu)
8 //results
9 printf("Bond anagle = %.2f degrees",2*u)
```

Scilab code Exa 6.4 Example 4

```
1 clc
2 //initialization of variables
3 cosu=1/sqrt(3)
4 sinu=sqrt(2/3)
5 //calculations
6 f=1/2 + sqrt(3) /2 *cosu + sqrt(3/2) *sinu
7 //results
8 printf("Pauling strength = %d ",f)
```

Scilab code Exa 6.5 Example 5

```
1 clc
2 //initialization of variables
3 alpha=60
4 //calculations
5 cosa=cosd(alpha)
6 sina=sind(alpha)
7 //results
8 printf("Wave function = %.2f s + %.2f pz",cosa,sina
    )
```

Scilab code Exa 6.9 Example 9

```
clc
//initialization of variables
DHH=103 //kcal/mol
//calculations
DHHp=0.5*(DHH)
//results
printf("Bond energy = %.1f kcal/mol",DHHp)
```

Scilab code Exa 6.10 Example 10

```
clc
//initialization of variables
DHH=42 //kcal/mol
//calculations
DHHp=0.5*(DHH)
//results
printf("Exchange energy = %.1f kcal/mol",DHHp)
```

Chapter 7

Gases and Introductory stastical thermodynamics

Scilab code Exa 7.2 Example 2

```
clc
//Initialization of variables
h=76 //cm
d=13.5951 //g/cc
g=980.655 //cm/s^2
T=273.15 //K
v=22414.6 //cm^3 /mol
//calculations
P=h*d*g
R=P*v/(T)
//results
printf("Gas constant = %.3e ergs/deg. mol",R)
```

Scilab code Exa 7.3 Example 3

```
clc
```

```
2 //Initialization of variables
3 cal=4.184*10^7 //ergs
4 R=8.315*10^7 //ergs/deg/mol
5 //calculations
6 Rdash=R/cal
7 //results
8 printf("R in calories = %.3f cal/ deg mol",Rdash)
```

Scilab code Exa 7.4 Example 4

```
1 clc
2 //Initialization of variables
3 R=8.315*10^7 //ergs/deg/mol
4 T=273.2 //deg
5 M=4 //g/mol
6 //calculations
7 u2=3*T*R/M
8 u=sqrt(u2)
9 //results
10 printf("root mean square velocity = %.2e cm/sec",u)
```

Scilab code Exa 7.5 Example 5

```
1 clc
2 //Initialization of variables
3 n1=2
4 n2=10
5 n3=3
6 P=720 //mm of Hg
7 //calculations
8 n=n1+n2+n3
9 x1=n1/n
10 P1=x1*P
```

```
x2=n2/n
P2=x2*P
x3=n3/n
P3=x3*P
//results
printf("\n Partial pressure of N2 = %d mm",P1)
printf("\n Partial pressure of O2 = %d mm",P2)
printf("\n Partial pressure of CO2 = %d mm",P3)
```

Scilab code Exa 7.6 Example 6

```
clc
//Initialization of variables
T=273.2+25 //K
n=1 //mol
R=1.987 //cal/deg mol
//calculations
Etr=1.5*n*R*T
Erot=1.5*n*R*T
Evib=0
Eel=0
Etot=Etr+Erot+Evib+Eel
//results
printf("Total energy = %d cal",Etot)
```

Scilab code Exa 7.7 Example 7

```
clc
//Initialization of variables
b=24.1 //cm^2/mol
N=6.023*10^23 //mole^-1
//calculations
d=(3*b/(2*%pi*N))^(1/3)
```

```
7 //results
8 printf("Molecular diameter of He = %.2e cm",d)
```

Scilab code Exa 7.8 Example 8

```
1 clc
2 //Initialization of variables
3 P=100 //atm
4 T=200 //K
5 n=1 //mole
6 R=0.08206 //l atm/deg mol
7 disp("From psychrometric charts,")
8 Tc=126.2 //K
9 Pc=33.5 //K
10 //calculations
11 Pr=P/Pc
12 Tr=T/Tc
13 disp("From z charts,")
14 z=0.83
15 V=z*n*R*T/P
16 //results
17 printf("Volume = %.3f liter",V)
```

Chapter 8

First law of thermodynamics

Scilab code Exa 8.1 Example 1

```
1 clc
2 //Initialization of variables
3 P=1.0132*10^6 //dynes/cm^2
4 A=100 //cm^2
5 z=10 //cm
6 //calculations
7 w=P*A*z*10^-7
8 //results
9 printf("Joules = %.4e J",w)
```

Scilab code Exa 8.2 Example 2

```
1 clc
2 //Initialization of variables
3 P=1.0132*10^6 //dynes/cm^2
4 A=100 //cm^2
5 z=10 //cm
6 //calculations
```

```
w=P*A*z*10^-7
cal=w/4.184
//results
printf("Calories = %.3f cal",cal)
```

Scilab code Exa 8.3 Example 3

```
clc
//Initialization of variables
T=373.2 //K
n=1 //mol
qp=9720 //cal/mol
//calculations
q=n*qp
w=1.987*T
dE=q-w
//results
printf("Heat of vaporization = %d cal",q)
printf("\n Change in energy = %d cal",dE)
```

Scilab code Exa 8.4 Example 4

```
clc
//Initialization of variables
T1=25+273 //K
T2=25+273 //K
//calculations
disp("Since, T2=T1, dE=0")
dE=0
w=0
q=dE+w
//results
printf("\n Work done = %d ",w)
```

```
12 printf("\n Heat transferred = %d ",q)
13 printf("\n Change in energy = %d",dE)
```

Scilab code Exa 8.5 Example 5

```
1  clc
2  //Initialization of variables
3  R=1.987 //cal/deg mol
4  //calculations
5  Cvtr=1.5*R
6  Cvrot=1.5*R
7  Cvt=Cvtr+Cvrot
8  disp("Observed Cv= 6.43")
9  Cvobs=6.43
10 Cvvib=Cvobs-Cvt
11 //results
12 printf("Vibrational = %.2f cal/deg mol",Cvvib)
```

Chapter 9

Boltzmann distribution law

Scilab code Exa 9.1 Example 1

```
clc
//Initialization of variables
r=2.1*10^-6 //cm
n=889
x=0.1 //cm
T=298.2 //K
//calculations
V=4/3 *%pi *r^3
rho=19.3-1
ffd=rho*V*980.7
eps=ffd*x
logN=-6.96*10^-14 /(2.303*1.38*10^-16 *T)
N=10^logN *n
//results
printf("No. of particles = %d ",N+1)
```

Scilab code Exa 9.2 Example 2

```
clc
//Initialization of variables
x=1 //percent
wave=1595 //cm^-1
//calculations
E=2.8593*wave
Nratio=(100-x)/x
logN=log10(Nratio)
T=E/(2.303*1.987*logN)
//results
printf("Temperature = %d K",T)
```

Chapter 10

Second law of thermodynamics

Scilab code Exa 10.1 Example 1

```
clc
//Initialization of variables
T2=100+273.2 //K
T1=50+273.2 //K
n=1 //mol
R=1.987 //cal/deg mol
//calculations
dS=5/2 *n*R*2.303*log10(T2/T1)
//results
printf("Change in entropy = %.3f eu",dS)
```

Scilab code Exa 10.3 Example 3

```
clc
//Initialization of variables
H=380 //cal
T=273.2+32.1 //K
//calculations
```

```
dS=H/T
//results
printf("Entropy change = %.2f eu",dS)
```

Scilab code Exa 10.5 Example 5

```
clc
//Initialization of variables
Ha=0
Hb=0
//calculations
H=Ha+Hb
q=H
U=0
w=q-H
//results
printf("Work done = %d",w)
```

Scilab code Exa 10.6 Example 6

```
clc
//Initialization of variables
prob=0.001
R=1
N=6.023*10^23
//calculations
dS=1.987*2.303*log10(prob) /N
//results
printf("change in entropy = %.1e eu",dS)
```

Scilab code Exa 10.7 Example 7

```
clc
//Initialization of variables
T=373.2 //K
c=1.987 //cal/deg
//calculations
w=c*T
A=-w
//results
printf("Change in A = %d cal",A)
```

Chapter 11

Condensed phases

Scilab code Exa 11.1 Example 1

```
clc
//Initialization of variables
A=7.6546
B=1686.8
T=60+273.2
//calculations
logP=A-B/T
P=10^logP
//results
printf("Vapor Pressure = %d mm",P+1)
```

Scilab code Exa 11.2 Example 2

```
clc
//Initialization of variables
alpha=4.92*10^-5 //deg^-1
beta=7.85*10^-7 //atm^-1
d=8.93 //g/cm^3
```

```
T=298.15 //K
//calculations
dC=63.54*T*alpha^2 *1.987/(d*beta*82.06)
//results
printf("Change in c values = %.3f cal/deg mol",dC)
```

Chapter 12

Physical Equilibria

Scilab code Exa 12.1 Example 1

```
clc
//Initialization of variables
p=3
c=2
//calculations
f=2-p+c
//results
printf("no. of degrees of freedom = %d ",f)
```

Scilab code Exa 12.2 Example 2

```
clc
//Initialization of variables
T=273.2 //K
vw=1.0001 //cm^3 /g
vi=1.0907 //cm^3 /g
hf=79.7 //cal/g
P1=76 //cm
```

```
8 P2=4.6 //cm
9 //calculations
10 dT=T*(vw-vi)*(P2-P1)*13.6*980.7/(hf*4.184*10^7)
11 //results
12 printf("change in temperature = %.4f deg",dT)
```

Scilab code Exa 12.3 Example 3

```
1 clc
2 //Initialization of variables
3 V=6.84 //cm^3 /g
4 //calculations
5 dPbydT=-1.7*4.184*10^7 /(2.19*V*0.06*1.01*10^6)
6 //results
7 printf("dPbydT = %d atm/deg",dPbydT)
```

Scilab code Exa 12.4 Example 4

```
1 clc
2 //Initialization of variables
3 P=6  //atm
4 T=273.2+25 //K
5 P=23.8 //mm
6 V=0.018 //lt/mol
7 R=0.08206 //lt am/deg mol
8 //calculations
9 dPa=V*P*4536/(R*T*760)
10 Pa=dPa+P
11 //results
12 printf("Pressure = %.1f mm",Pa)
```

Scilab code Exa 12.5 Example 5

```
clc
//Initialization of variables
x=0.25
Ps1=96 //mm
Ps2=43.9 //mm
//calculations
P1=x*Ps1
P2=(1-x)*Ps2
P=P1+P2
Xdash=P1/P
//results
printf("mole fraction of methanol in vapor =%.3f ",
   Xdash)
```

Scilab code Exa 12.6 Example 6

```
clc
//Initialization of variables
Hv=539.6 //cal/g
T=273.2+100 //K
//calculations
Kb=1.987*T^2 /(1000*Hv)
//results
printf("Molal elevation constant =%.3f deg /mole /
   kg",Kb)
```

Scilab code Exa 12.7 Example 7

```
clc
//Initialization of variables
ms=0.5 //mol/kg
```

```
m=5 //g
mw=100 //g
Ws=1000 //g/kg
//calculations
Ma=m*Ws/(ms*mw)
//results
printf("Molecular weight of solute = %d g/mol ",Ma)
```

Scilab code Exa 12.8 Example 8

```
clc
//Initialization of variables
dT=0.23 //C
Kb=1.86 //deg/mol/kg
//calculations
m=dT/Kb
//results
printf("molality of solution = %.2f m",m)
```

Scilab code Exa 12.9 Example 9

```
clc
//Initialization of variables
p=0.1 //m
T=30+273.2  //K
R=0.08206 //lt atm /deg/mol
P1=1 //atm
//calculations
w=1000/p
V=w/1000
dP=R*T/V
P=dP+P1
//results
```

```
13 printf("Osmotic Pressure =%.2f atm ",P)
```

Chapter 13

Thermodynamic changes accompanying chemical reaction

Scilab code Exa 13.1 Example 1

```
1 clc
2 //Initialization of variables
3 n1=10 //mol
4 n2=12 //mol
5 //calculations
6 dn=n1-n2
7 //results
8 printf("dHp = dEv- %d *RT",dn)
```

Scilab code Exa 13.2 Example 2

```
1 clc
2 //Initialization of variables
3 Ht1=-22063 //cal
```

```
4 T=298.15 //K
5 //calculations
6 H=Ht1 +0.5293*T + 0.3398*10^-3 *T^2 - 2.039*10^-7 *T
     ^3
7 //results
8 printf("Enthalpy = %d cal",H)
```

Scilab code Exa 13.3 Example 3

```
1 clc
2 //Initialization of variables
3 Cp=0.797 //cal/deg/mol
4 //calculations
5 S=Cp/3
6 //results
7 printf("Entropy = %.3f eu/mol",S)
```

Scilab code Exa 13.4 Example 4

```
1 clc
2 //Initialization of variables
3 T1=77.32 //K
4 P=1 //atm
5 T2=126 //K
6 Pc=33.5 //atm
7 //calculations
8 dS=27/32 *1.987*P/Pc *(T2/T1)^3
9 //results
10 printf("Change in entropy = %.2f eu/mol",dS)
```

Scilab code Exa 13.5 Example 5

```
clc
//Initialization of variables
S1=57.47
S2=50.34
S3=49
H1=8.09
H2=21.06
H3=0
F1=12.39
F2=20.72
F3=0
//calculations
dS=S1-S2-0.5*S3
dH=H1-H2-0.5*H3
dF=F1-F2-0.5*F3
//results
printf("Change in entropy = %.2f eu",dS)
printf("\n Change in enthalpy = %.2f kcal",dH)
printf("\n Change in free energy = %.2f kcal",dF)
```

Scilab code Exa 13.6 Example 6

```
clc
//Initialization of variables
P1=0.01
P2=0.1
P3=0.01
dF0=-54640 //cal
T=298.15 //K
R=1.987 //cal/deg
//calculations
Qp=P1/(P2*P3^0.5)
dF=dF0+R*T*log(Qp)
```

```
12 //results
13 printf("change in free energy = %d cal",dF)
```

Scilab code Exa 13.7 Example 7

```
1 clc
2 //Initialization of variables
3 disp("From table 13.4 ")
4 logKfwater=40.04724
5 logKfH2=0
6 logKfO2=0
7 //calculations
8 logK=logKfwater-logKfH2-0.5*logKfO2
9 K=10^logK
10 //results
11 printf("Equilibrium constant = %.4e",K)
```

Scilab code Exa 13.8 Example 8

```
1 clc
2 //Initialization of variables
3 Kp=1.1*10^40 //atm^-0.5
4 dn=-0.5
5 R=0.08206 //lt atm/deg mol
6 T=298.15 //K
7 //calculations
8 Kc=Kp*(R*T)^(-dn)
9 //results
10 printf("Kc = %.1e (mol/lt)^-0.5",Kc)
```

Scilab code Exa 13.9 Example 9

```
clc
//Initialization of variables
Kp=0.141 //atm
P=1 //atm
nu=2
R=0.08206 //lt atm/deg mol
T=298.15 //K
M=92.02 //g/mol
//calculations
a=poly(0,"a");
p=Kp*a^2 +4*a^2*P -Kp
z=roots(p)
alpha=z(1)
wbyV=P*M/(R*T*(1+(nu-1)*alpha))
//results
printf("Density of the equilibrium mixture = %.2f g/
   lt",wbyV)
```

Scilab code Exa 13.10 Example 10

```
clc
//Initialization of variables
x=0.5
P=0.468 //atm
//calculations
P1=x*P
P2=x*P
Kp=P1*P2
//results
printf("Final pressure after quilibrium = %.4f atm^2
   ",Kp)
```

Chapter 14

Development and use of activity concepts

Scilab code Exa 14.1 Example 1

```
1 clc
2 //Initialization of variables
3 x1=0.0200
4 Kx=812
5 //calculations
6 disp("Neglecting 2x in comparision with x1,")
7 x=x1/Kx
8 //results
9 printf("Moles of Iodine present = %.2e mole",x)
```

Scilab code Exa 14.2 Example 2

```
1 clc
2 //Initialization of variables
3 Kc=1.749*10^-5 //M
4 n1=0.1 //mole
```

```
n2=0.01 //mole
//calculations
c=n1/n2 *Kc
//results
printf("Concentration of Hplus ions = %.1e M",c)
```

Scilab code Exa 14.3 Example 3

```
clc
//Initialization of variables
c=0.01 //M
kc=1.749*10^-5 //M
//calculations
x2=c*kc
x=sqrt(x2)
//results
printf("Concentraton of Hplus ions = %.1e M",x)
```

Scilab code Exa 14.4 Example 4

```
clc
//Initialization of variables
K2=1.0008*10^-14 //m^2
K1=1.754*10^-5 //m
c=0.1
//calculations
disp("Neglecting x w.r.t c,")
x2=c*K2/K1
x=sqrt(x2)
//results
printf("Concentration of OH minus ions = %.1e m",x)
```

Scilab code Exa 14.5 Example 5

```
clc
//Initialization of variables
disp("from table 14.1,")
r1=7.47*10^-5 //m
r2=4.57*10^-3 //m
mp=1.008*10^-14 //m^2
//calculations
r3=r2/r1
mH2=r3*mp
mH=sqrt(mH2)
//results
printf("Concentraton of Hplus ions = %.2e M",mH)
```

Scilab code Exa 14.6 Example 6

```
clc
//Initialization of variables
disp("from table 14.1,")
r1=1.75*10^-5 //m
r2=1.772*10^-4 //m
mp=1.008*10^-14 //m^2
//calculations
r3=r2/r1
mH2=r3*mp
mH=sqrt(mH2)
//results
printf("Concentraton of Hplus ions = %.1e M",mH)
```

Scilab code Exa 14.7 example 7

```
clc
//Initialization of variables
c=1*10^-6 //m
K=1.754*10^-5 //m
Kp=1.008*10^-14 //m^2
//calculations
mH=c
//Iteration 1
mOH=Kp/mH
mA=mH-mOH
mHA=mH*mA/K
mH2=mH-mHA+mOH
//Iteration 2
mOH2=Kp/mH2
mA2=mH2-mOH2
mHA2=mH2*mA2/K
mH3=mH2-mHA2+mOH2
//From x2
x2=sqrt(Kp)
x1=c
mOH3=Kp/x2
y2=x1
//From x1
mOH4=Kp/c
mA4=mH-mOH4
mHA4=mH*mA4/K
y1=c-mHA4-mA4
//upon further iterations, we get
mHplus=mH3
//results
printf("Concentration of H plus ions = %.2e m",
   mHplus)
//The answer is a bit different due to rounding off
   error.
```

Scilab code Exa 14.8 Example 8

```
clc
//Initialization of variableH
disp("From table 14-3,")
HH=0
HHcoo=-98
HHcooh=-98
SH=0
SHcoo=21.9
SHcooh=39.1
KH=0
KHcoo=58.64
KHcooh=62.38
//calculationH
dH=HH+HHcoo-HHcooh
dS=SH+SHcoo-SHcooh
dK=KH+KHcoo-KHcooh
K=10^dK
//results
printf(" dS0 = %.1f eu",dS)
printf("\n dH0 = %.1f kcal",dH)
printf("\n log Krm = %.2f ",dK)
printf("\n Krm = %.1e m",K)
```

Scilab code Exa 14.9 Example 9

```
clc
//Initialization of variables
mca=0.01 //m
mcl=0.02 //m
//calculations
```

```
Mu=0.5*(mca*4 + mcl*1)
disp("From table 14-5,")
aca=6 //A
acl=3 //A
disp("From table 14-6,")
gaca=0.555
gacl=0.843
Aca=gaca*mca
Acl=gacl*mcl
//results
printf("Activity of cl = %.4f ",Acl)
printf("\n Activity of ca = %.4f ",Aca)
```

Scilab code Exa 14.10 Example 10

```
clc
//Initialization of variables
m1=0.1 //m
m2=0.1 //m
K=1.754*10^-5 //m
//calculations
mu=0.5*(m1*1^2 + m2*1^2)
disp("From table 14.5,")
aH=9 //A
aA=4.5 //A
disp("From table 14.6")
gH=0.825
gA=0.775
gHA=1
x1=gHA*K/(gH*gA)
disp("Assuming x to be small w.r.t m1,")
x=sqrt(x1*m1)
//results
printf("Concentration of H plus ions = %.2e m",x)
```

Scilab code Exa 14.11 Example 11

```
clc
//Initialization of variables
K=1.754*10^-5 //m
c=0.1
//calculations
disp("Neglecting x w.r.t c,")
x2=K
x=sqrt(K)
mu=x
disp("From tables 14-5 and 14-6,")
gH=0.963
gA=0.960
x22=K/(gH*gA)
a=poly(0,"a");
p=a^2 +a*x22 -c*x22
z=roots(p)
alpha=z(2)
//results
printf("concentration of H plus ions = %.2e m",alpha
   )
```

Scilab code Exa 14.12 Example 12

```
clc
//Initialization of variables
disp("From table 14.3")
K1=-13.5089
K2=-22.9792
K3=19.2218
c=0.1 //m
```

```
8 //calculations
9 logK=K1-K2-K3
10 K=10^logK
11 mu=0.5*(c*1^2 + c*1^2)
12 disp("From tables 14-5 and 14-6,")
13 gAg=0.745
14 gCl=0.755
15 x2=K/(gAg*gCl)
16 x=sqrt(x2)
17 //results
18 printf("Solubility of Agcl = %.2e m",x)
```

Scilab code Exa 14.13 Example 13

```
1 clc
2 //Initialization of variables
3 Cna=0.11
4 Ccl=0.1
5 //calculations
6 x=poly(0,"x");
7 p=99*x^2 - 2.1*x+Cna*Ccl
8 z=roots(p)
9 alpha=z(2)
10 Na1=Cna-10*alpha
11 Cl1=Ccl-10*alpha
12 //results
13 printf(" Concentration of Na in 1 = %.4f M",Na1)
14 printf("\n Concentration of Cl in 1 = %.4f M",Cl1)
15 printf("\n Concentration of Na in 2 = %.4f M",alpha
   )
16 printf("\n Concentration of Cl in 2 = %.4f M",alpha
   )
```

Chapter 15

Electrochemistry

Scilab code Exa 15.1 Example 1

```
clc
//Initialization of variables
I=0.5 //amp
t=55  //min
we=31.77
//calculations
Q=I*t*60
n=Q/96496
w=n*we
//results
printf("Weight of copper leaving = %.3f g",w)
```

Scilab code Exa 15.2 Example 2

```
clc
//Initialization of variables
w1=0.7532 //g
w2=0.9972 //g
```

```
wdep=0.4 //g
we=31.77 //g
//calculations
dn=w2/we - w1/we
t=dn/(wdep/we)
dne=wdep/we
dnmig=dn-dne
tplus=-dnmig/dne
tminus=1-tplus
//results
printf("tplus = %.3f",tplus)
printf("\n tminus= %.3f",tminus)
```

Scilab code Exa 15.3 Example 3

```
clc
//Initialization of variables
R1=312 //ohms
R2=1043 //ohms
c=0.01 //N
kdash=0.002768 //ohm^-1cm^-1
//calculations
k=kdash*R1
kdash2=k/R2
lambda=kdash2/(c/1000)
//results
printf("Equivalent conductance = %.1f ohm^-1 cm^2
   equiv^-1",lambda)
```

Scilab code Exa 15.4 Example 4

```
clc
//Initialization of variables
```

```
3 l1=349.8
4 l2=40.9
5 //calculations
6 l=l1+l2
7 //results
8 printf("Conductance for acetic acid = %.1f ohm^-1 cm
    ^2",l)
```

Scilab code Exa 15.5 Example 5

```
1 clc
2 //Initialization of variables
3 l1=63.6
4 l2=79.8
5 n=1 //mg/lt
6 we=116.7 //g/equiv
7 //calculations
8 l=l1+l2
9 c=n*10^-3 /we
10 k=c*l/1000
11 //results
12 printf("Specific conductance = %.2e ohm^-1 cm^-1",k)
```

Scilab code Exa 15.6 Example 6

```
1 clc
2 //Initialization of variables
3 e1=0.763 //volt
4 e2=0.337 //volt
5 //calculations
6 e0=e1+e2
7 //results
```

```
8 printf("Standard electrode potential of the cell = %
    .3f volts",e0)
```

Scilab code Exa 15.7 Example 7

```
1  clc
2  //Initialization of variables
3  aZn=0.1
4  aCu=0.01
5  e1=0.763 //volt
6  e2=0.337 //volt
7  //calculations
8  e0=e1+e2
9  Q=aZn/aCu
10 E=e0- 0.05915*log10(Q) /2
11 //results
12 printf("Emf of the cell = %.3f volts",E)
```

Chapter 16

Typical mechanisms and rate laws

Scilab code Exa 16.1 Example 1

```
clc
//Initialization of variables
P1=69.2 //mm
P2=39.8//mm
t=20 //min
//calculations
k=2.303*log10(P1/P2) /(t*60)
//results
printf("Rate constant = %.2e sec^-1",k)
```

Scilab code Exa 16.2 Example 2

```
clc
//Initialization of variables
t=10 //min
x=90
```

```
5 //calculations
6 k=2.303*log10(100/(100-x)) /t
7 //results
8 printf("Rate constant = %.3f min^-1",k)
```

Scilab code Exa 16.3 Example 3

```
1 clc
2 //Initialization of variables
3 t=242 //sec
4 P=229 //mm
5 P0=363 //mm
6 //calculations
7 k=(1/P -1/P0)/t
8 //results
9 printf("rate constant= %.2e sec^-1 mm^-1",k)
```

Chapter 17

Resolving Kinetic data

Scilab code Exa 17.1 Example 1

```
clc
//Initialization of variablesx1=5
x2=20
x1=5
n1=7.49
n2=5.14
//calculations
n=(log(n1)-log(n2))/(log(100-x1) - log(100-x2))
//results
printf("Order of the reaction  = %.2f",n)
```

Scilab code Exa 17.2 Example 2

```
clc
//Initialization of variables
p2=169
p1=363
t1=410
```

```
t2=880
//calculations
ndash=(log(t2) - log(t1))/(log(p1) - log(p2))
n=ndash+1
//results
printf("Order of the reaction = %.2f",n)
```

Scilab code Exa 17.3 Example 3

```
clc
//Initialization of variables
R=1.987 //cal/deg/mol
k1=4.45*10^-5
k2=2.52*10^-6
T1=283+273.2 //K
T2=356+273.2 //K
//calculations
Ea=2.303*R*1.7530 /(1/T1 - 1/T2)
logZ= log10(k1) +Ea/(2.303*R*T1)
Z=10^logZ
//results
printf("Activation energy = %d cal/mol",Ea)
printf("\n Z = %.1e lt /mol sec",Z)
```

Scilab code Exa 17.5 Example 5

```
clc
//Initialization of variables
g1=0.661
g2=0.899
g3=0.405
g4=0.803
g5=0.946
```

```
g6=0.614
k=1.33
//calculations
k0=k*g3/(g1*g2)
k2=k0*g4*g5/g6
//results
printf("Equlibrium constant = %.2f lt/mol min",k2)
```

Chapter 18

Catalysis

Scilab code Exa 18.1 Example 1

```
clc
//Initialization of variables
V1=0.284 //cm^3 /g
V2=1.43 //cm^3 /g
P1=142.4 //mm
P2=760 //mm
//calculations
z=(1/V1 - 1/V2)/(1/P1 - 1/P2)
invVm=1/V2 - z/P2
Vm=1/invVm
//results
printf("Volume = %.1f cm^3/g",Vm)
//The answer in the textbook is a bit different due
   to rounding off error.
```

Scilab code Exa 18.2 Example 2

```
clc
```

```
2 //Initialization of variables
3 Vm=2.86 //cc/g
4 P=1 //atm
5 R=82.06 //cm^3 atm/deg mol
6 T=273.2 //deg
7 N=6.023*10^23
8 sigma=16.2*10^-16 //cm^2 /molecule
9 //calculations
10 n=P*Vm/(R*T)
11 A=N*n*sigma
12 //results
13 printf("total area = %.2e cm^2 (g catalyst)^-1",A)
```

Chapter 19

Photochemistry

Scilab code Exa 19.1 Example 1

```
clc
//Initialization of variables
r1=0.727
r2=0.407
//calculations
r3=r1*r2
//results
printf("Overall transmittance = %.3f",r3)
```

Scilab code Exa 19.2 Example 2

```
clc
//Initialization of variables
r=0.450
c=0.02 //M
l=4 //cm
//calculations
e=-log10(r) /(c*l)
```

```
8 //results
9 printf("Extinction coefficient = %.2f litres mole^-1
      cm^-1",e)
```

Scilab code Exa 19.3 Example 3

```
1 clc
2 //Initialization of variables
3 r1=0.850
4 r2=0.50
5 //calculations
6 Da=-log10(r1)
7 Db=-log10(r2)
8 D=Da+Db
9 r3=10^(-D)
10 //results
11 printf("Transmittance of solution = %.3f ",r3)
```

Scilab code Exa 19.4 Example 4

```
1 clc
2 //Initialization of variables
3 c=0.000025 //M
4 l=2 //cm
5 D=0.417
6 //calculations
7 e=D/(c*l)
8 //result
9 printf("Extinction coefficient = %d liters mole^-1
     cm^-1",e)
```

Scilab code Exa 19.5 Example 5

```
clc
//Initialization of variables
c=0.5 //M
c1=0.000025 //M
D2=0.280
D1=0.417
//calculations
c2=D2*c1/(D1)
dC=c1-c2
SCN=c- 6*c2 -4*dC
K=dC*SCN^2 /c2
//results
printf("Kc for dissociation = %.2f M^2",K)
```

Scilab code Exa 19.6 Example 6

```
clc
//Initialization of variables
D2=0.249
D1=0.172
a2=0.00752
a1=0.00527
//calculations
m=(log(D2) -log(D1))/(log(a2) - log(a1))
//results
printf("m = %.2f ",m)
```

Scilab code Exa 19.7 Example 7

```
clc
//Initialization of variables
```

```
c=0.1 //M
V=100 //ml
v1=25 //ml
D=0.980
d1=0.090
d2=0.150
//calculations
a=v1*c/V
b=(V-v1)*c/V
Da=a*d1/c
Db=b*d2/c
Ddash=Da+Db
dD=D-Ddash
//results
printf("Increase in optical density = %.3f",dD)
```

Scilab code Exa 19.8 Example 8

```
clc
//Initialization of variables
E=50000 //cal/mol
//calculations
lam=2.8593/E
//results
printf("For the reaction to occur lambda < %d A",lam
   *10^8)
```

Scilab code Exa 19.9 Example 9

```
clc
//Initialization of variables
lam=3000*10^-8 //cm
yield=0.420
```

```
5  Et=70000 //cal
6  //calculations
7  E=2.8593/lam
8  n=yield*Et/E
9  //results
10 printf("Amount of reactant disappeared = %.3f mol",n
     )
```