Scilab Textbook Companion for Elements Of Physical Chemistry by P. Atkins[1]

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Book Description

Title: Elements Of 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

The properties of gases

Scilab code Exa 1.1.e example 1

```
clc
//Initialzation of variables
m=1.25 //g
MN2=28.02 //g/mol
T=20+273.15 //K
V=0.25//L
//Calculations
P=m*8.31451*T/(MN2*V)
//Results
printf('Pressure in the gas flask =%.2f kPa',P)
```

Scilab code Exa 1.2.i illustration 2

```
clc
//Initialzation of variables
xN2=0.780
xO2=0.210
xAr=0.009
```

```
P=100 //kPa
//Calculations
PN2=xN2*P
PO2=xO2*P
PAr=xAr*P
//Results
printf('Partial pressure of Nitrogen(kPa) = %.1f',
   PN2)
printf('\n Partial pressure of Oxygen(kPa) = %.1f',
   PO2)
printf('\n Partial pressure of Argon(kPa) = %.1f',
   PAr)
```

Scilab code Exa 1.3.i Illustration 3

```
clc
//Initialzation of variables
T1=298//K
T2=273//K
//Calculations
factor=sqrt(T2/T1)
percentage=(1-factor)*100
//Results
printf('Percentage loss of speed of air molecules =
   %.2f',percentage)
```

Scilab code Exa 1.4.i illustration 4

```
clc
//Initialzation of variables
MH2=2.016 //g/mol
MCO2=44.01 //g/mol
//calculations
```

```
ratio=sqrt(MCO2/MH2)
//results
printf('ratio of rates of effusion =%.3f',ratio)
```

Scilab code Exa 1.5.i illustration 5

```
clc
//Initialzation of variables
T=25+273 //K
sigma=0.4*10^(-18) //m^2
P=10^5 //Pa
c=481.8 //m/sec
//Calculations
Lambda=8.31451*T/(2^0.5 *6.022*10^23 *sigma*P)
frequency=2^0.5 *6.022*10^23 *sigma*P*c/(8.31451*T)
//Results
printf('Mean free path = %.2e m',Lambda)
printf('\n Collision frequency = %.2e m',frequency)
```

Chapter 2

Thermodynamics The first law

Scilab code Exa 2.1.e example 1

```
clc
//Initialization of variables
A=1.23 //A
V=12 //V
t=123 //s
Temp=4.47 //C
rise=3.22 //C
//Calculations
q=A*V*t
C=q/Temp
Output= C*rise
//Results
printf('heat supplied during calibration = %.1f J',q
   )
printf('\n Heat capacity of the calorimeter = %.1f J
   /C',C)
printf('\n Heat output = %.2f kJ',Output/1000.)
```

Scilab code Exa 2.1.i illustration 1

```
clc
//Initialization of variables
Cpm=75 //J/k mol
n=5.55 //mol
q=1 //kJ
//Calculations
deltaT=q*1000/(n*Cpm)
//results
printf('Change in temperature = %.1f K',deltaT)
```

Scilab code Exa 2.2.e example 2

```
clc
//Initialization of variables
work=-622 //kJ
heat=-82 //kJ
//Calculations
U=work+heat
//results
printf('The persons internal energy falls by %d kJ',
   U)
```

Scilab code Exa 2.4.i illustration 4

```
clc
//Initialization of variables
n=5.55 //mol
T1=20 //C
T2=80 //K
Cpm=75.29 //J/K mol
//Calculations
H=n*Cpm*(T2-T1)
//results
```

```
10 printf('Enthalpy of the sample changes by %d kJ',H
   /1000.)
```

Chapter 3

Thermochemistry

Scilab code Exa 3.1.e example 1

```
clc
//Initialization of variables
I=0.682 //A
V=12 //V
t=500 //s
m=4.33 //g
MW=46.07 //g/mol
//Calculations
q=I*V*t
n=m/MW
H=q/n
//Results
printf('Molar enthalpy change = %.1f kJ/mol',H
   /1000.)
```

Scilab code Exa 3.1.i illustration 1

```
clc
```

```
2 //Initialization of variables
3 dU=-969.6 //kJ/mol
4 nN2=1/2
5 nCO2=2
6 nO2=9/4
7 T=298.15 //K
8 //Calculations
9 n=nCO2+nN2-nO2
10 H=dU+n*8.3145*T/1000.
11 //results
12 printf('Enthalpy change =%.1f kJ/mol',H)
```

Scilab code Exa 3.2.e example 2

```
1 clc
2 //Initialization of variables
3 m=1 //g
4 MW=24.31 //g/mol
5 H=2337 //kJ/mol
6 //Calculations
7 n=m/MW
8 q=n*H
9 //results
10 printf('Heat supplied = %.1f kJ',q)
```

Scilab code Exa 3.3.e example 3

```
1 clc
2 //Initialization of variables
3 HC=716.68 //kJ
4 HH=871.88 //kJ
5 HO=249.17 //kJ
6 Hcond=-38 //kJ
```

```
HCH=-412
HCO=-360
HOH=-463
//Calculations
H1=HC+HH+HO
H2=3*HCH+HCO+HOH
H3=Hcond
H=H1+H2+H3
//results
printf('Sum of enthalpy changes = %d kJ',H)
```

Scilab code Exa 3.4.e example 4

```
clc
//Initialization of variables
Hf=-124 //kJ
Hoxi=-2220 //kJ
Hwater=286 //kJ
//Calculations
H=Hf+Hoxi+Hwater
//results
printf('Standard enthalpy of combustion of propene =
    %d kJ/mol',H)
```

Scilab code Exa 3.5.e Example 5

```
clc
//Initialization of variables
nCO2=6 //mol
nH2O=3 //mol
nO2=15/2 //mol
nC6H6=1 //mol
HC6H6=49 //kJ/mol
```

```
HH2O=-285.83
HO2=0
HCO2=-393.51
//Calculations
H=nCO2*HCO2+nH2O*HH2O-nC6H6*HC6H6-nO2*HO2
//results
printf('Standard enthalpy of combustion of benzene
    is %d kJ/mol',H-1)
```

Scilab code Exa 3.6.e example 6

```
clc
//Initialization of variables
HH2O=-241.82 //kJ/mol
T1=25 //C
T2=100 //C
CpH2O=33.58 //J/K mol
CpH2=28.84 //J/K mol
CpO2=29.37  //J/K mol
//calculations
dCp=CpH2O-CpH2-0.5*CpO2
dH=HH2O+dCp*(T2-T1)/1000.
//results
printf('Enthalpy of fromation of water at 100 C is %
    .2f kJ/mol',dH)
```

Chapter 4

Thermodynamics The second law

Scilab code Exa 4.1.e example 1

```
1  clc
2  //Initialization of variables
3  Power=100 //W
4  time=1 //day
5  T=20 //C
6  //calculations
7  timeins=1*24*3600
8  qsurr=timeins*Power
9  Ssurr=qsurr/(T+273)
10 //results
11 printf('Heat transferred to surroundings = %d J',
       qsurr)
12 printf('\n Entropy production per day = %.2e J/k',
       Ssurr)
```

Scilab code Exa 4.1.i illustration 1

```
clc
//Initialization of variables
H=100 //kJ
T1=273 //K
T2=373//K
//calculations
S1=H*1000/T1
S2=H*1000/T2
//results
printf('Entropy change at 273 K is %d J/K ',S1)
printf('\n Entropy change at 373 K is %d J/K ',S2)
```

Scilab code Exa 4.2.e example 2

```
clc
//Initialization of variables
g=9.81 //m/s^2
m=30*10^-3 //kg
d=10 //m
H=2.828*10^6 //j/mol
M=180 //g/mol
//calculations
w=g*m*d
n=w/H
m=n*M
//results
printf('Amount bird must consume = %.1e g',m)
```

Scilab code Exa 4.2.i illustration 2

```
clc
//Initialization of variables
T=59.2 //K
```

```
4 //calculations
5 Hvap=85*(273.2+T)
6 //results
7 printf('Enthalpy of vaportization  =%d kJ/mol',Hvap
    /1000)
```

Scilab code Exa 4.3.i illustration 3

```
1 clc
2 //Initialization of variables
3 SH2O=70 //J/K mol
4 SH2=131 //J/K mol
5 SO2=205 //J/K mol
6 //calculations
7 deltaS=2*SH2O-2*SH2-SO2
8 printf('Change in entropy = %d J/K mol',deltaS)
```

Chapter 6

The properties of mixtures

Scilab code Exa 6.1.e example 1

```
clc
//Initialization of variables
m=0.14 //mol/kg
w=1 //kg Assume
//Calculations
ngly=m*w
nwater=w*10^3 /18.02
ntotal=ngly+nwater
xgly=ngly/ntotal
//results
printf('Mole fraction of glycerine  is xgly = %.2e',
   xgly)
```

Scilab code Exa 6.2.e example 2

```
clc
//Initialization of variables
mE=50 //g
```

```
4  mW=50 //g
5  //calculations
6  nE=mE/46
7  nW=mW/18
8  ntotal=nE+nW
9  xE=nE/ntotal
10 xW=1-xE
11 disp('for the observed xE and xW')
12 vE=55 //cc/mol
13 vW=18 //cc/mol
14 V=nE*vE+nW*vW
15 //results
16 printf('\n VOlume of the mixture = %d cm^3 ',V+1)
```

Scilab code Exa 6.3.e example 3

```
1  clc
2  //Initialization of variables
3  xc=[0 0.20 0.40 0.60 0.80 1]
4  pc=[0 35 82 142 219 293]
5  pa=[347 270 185 102 37 0]
6  //calculations
7  plot(xc,pc)
8  plot(xc,pa)
9  xlabel('Mole fraction xc')
10 ytitle('Pressure /Torr')
11 disp('From the graph it is clear that KA=175 torr
      and KC=165 torr. They are plotted with Raoults
      law lines')
```

Scilab code Exa 6.4.e example 4

```
1  clc
```

```
2 //Initialization of variables
3 C=4 //mg/L
4 MO2=32 //g/mol
5 Mw=18
6 w=1 //L
7 K=3.3*10^7 //torr
8 patm=0.21*760 //torr
9 //calculations
10 nO2=C/MO2
11 nH2O=w*10^3 /Mw
12 xO2=nO2/(nO2+nH2O)
13 pO2=xO2*K
14 if(pO2>patm)
15     disp('The required concentration can be
       maintained under normal conditions')
16 else
17     disp('The required concentration cannot be
       maintained under normal conditions')
18 end
```

Scilab code Exa 6.5.e example 5

```
1 clc
2 //Initialization of variables
3 c=[1 2 4 7 9]
4 hbyc=[0.28 0.36 0.503 0.739 0.889]
5 R=8.3145 //J/K mol
6 T=298 //K
7 g=9.81 //m/s^2
8 d=0.9998 //g/cm^3
9 //calculations
10 plot(c,hbyc)
11 xlabel('c')
12 ylabel('hbyc')
13 vector=regress(c,hbyc)
```

```
14 intercept=vector(1)
15 intercept=intercept*10^-2
16 M=R*T/(d*g*intercept)
17 //results
18 printf('Molar mass of the enzyme is close to %d kDa'
      ,M/1000 -3)
```

Scilab code Exa 6.6.e example 6

```
1  clc
2  //Initialization of variables
3  nB=0.59 //mol
4  nNB=0.41 //mol
5  xN1=0.38
6  xN2=0.74
7  xNm=0.41
8  //calculations
9  disp('By lever rule')
10 ratio=(xNm-xN1)/(xN2-xNm)
11 percent=ratio*100
12 //results
13 printf("The rich phase is %d times more abundant in
      nitrobenzene",percent+1)
```

Chapter 7

Principles of chemical equilibrium

Scilab code Exa 7.1.e example 1

```
clc
//Initialization of variables
G=-31 //kJ/mol
T=37+273 //K
Cadp=10^-3 //mmol/L
Cp=8*10^-3 //mmol/L
Catp=8*10^-3 //mmol/L
R=8.314 //J/K mol
//calculations
Q=Cadp*Cp/Catp
deltaG=G+R*T*log(Q) /1000.
//results
printf("Reaction Gibbs energy = %d kJ/mol",deltaG-1)
```

Scilab code Exa 7.2.e example 2

```
clc
//Initialization of variables
Hr=-285.83 //kJ/mol
Sr=-163.34 //J/ K mol
T=298.15 //K
//calculations
Gr=Hr-T*Sr/1000.
//results
printf('Gibbs energy = %.2f kJ/mol',Gr)
```

Scilab code Exa 7.2.i illustration 2

```
clc
//Initialization of variables
Gr=-3.40 //kJ/mol
R=8.314 //J/k mol
T=298 //K
//calculations
lnK=Gr*10^3/(R*T)
K=exp(lnK)
//results
printf('Equilibrium constant K= %.2f',K)
```

Scilab code Exa 7.3.e example 3

```
clc
//Initialization of variables
aADP=1 //mol/L
aP=1 //mol/L
aATP=1 //mol/L
aH2O=1 //mol/L
aH=10^-7 //mol/L
G=10 //kJ/mol
```

```
T=298 //K
R=8.314 //J/K mol
//calculations
Q=aADP*aP*aH/(aATP*aH2O)
Gr=G+R*T*log(Q)/1000.
//results
printf('Change in nGibbs energy =%d kJ/mol',Gr-1)
```

Scilab code Exa 7.3.i illustration 3

```
clc
//Initialization of variables
Hr=178 //kJ/mol
Sr=161 //J/K mol
//calculations
T=Hr*10^3 /Sr
//results
printf("Decompostion temperature = %.2e K",T)
```

Scilab code Exa 7.4.e example 4

```
clc
//Initialization of variables
Gr=1.7*10^3 //J/mol
T=298 //K
R=8.314 //J/K mol
K=0.5
//calculations
GbyRT=Gr/(R*T)
feq=K/(K+1)
//results
printf("Equivalent fraction = %.2f ",feq)
disp("For the second part, Gr=1.7 + 2.48 ln(f/1-f)")
```

Scilab code Exa 7.4.i illustration 4

```
clc
//Initialization of variables
GCO2=-394 //kJ/mol
GCO=-137 //kJ/mol
GO2=0
//calculations
deltaG=2*GCO2-2*GCO+GO2
//results
printf('Standard reaction gibbs energy = %d kJ/mol',
   deltaG)
```

Scilab code Exa 7.5.e example 5

```
clc
//Initialization of variables
species=['N2' 'H2' 'NH3']
change=['-x' '-3x' '2x']
E=['1-x' '3-3x' '2x']
disp("Concentration table")
disp(species)
disp(change)
disp(E)
K=977
//Calculations
g=sqrt(27*K/4)
x=poly(0,'x');
vector=roots(g*x^2 -(2*g +1)*x +g)
sol=vector(2)
PN2=1-sol
```

```
17 PH2=3-3*sol
18 PNH3=2*sol
19 K=PNH3^2/(PH2^3 *PN2)
20 //results
21 printf("Pressure of N2 gas =%.2f bar",PN2)
22 printf("\n Pressure of H2 gas =%.2f bar",PH2)
23 printf("\n Pressure of NH3 gas =%.2f bar",PNH3)
24 printf("\n K final = %.1e> it is close to original
   value.",K)
```

Chapter 8

Consequences of equilibrium

Scilab code Exa 8.1.e example 1

```
clc
//Initialization of variables
C=0.15 //M
Ka=1.8*10^-5
//calculations
x=sqrt(C*Ka)
f=x/C
percent=f*100
//results
printf("percent of acetic acid molecules that have
   donated a proton = %.1f percent",percent)
```

Scilab code Exa 8.1.i illustration 1

```
clc
//Initialization of variables
ph1=6.37
ph2=10.25
```

```
ph3=7.21
ph4=12.67
//calculations
pH1=0.5*(ph1+ph2)
pH2=0.5*(ph3+ph4)
//results
printf("Equilibrium pH in case 1 = ",pH1)
printf("\n Equilibrium pH in case 2 = ",pH2)
```

Scilab code Exa 8.2.e example 2

```
clc
//Initialization of variables
pKa=4.88
C=0.01 //M
pKw=14
//calculations
pKb=pKw-pKa
Kb=10^(-pKb)
x=(sqrt(C*Kb))
pOH=-log(x)
pH=14-pOH
f=x/C
//results
printf("fraction protonated = %.1e",f)
printf("\n 1 molecule in about %d",1/f)
```

Scilab code Exa 8.2.i illustration 2

```
clc
//Initialization of variables
n=2.5*10^-3 //mol
C=0.2 //mol/L
```

```
5 vbase=37.5*10^-3 //L
6 //calculations
7 V=n/C
8 base=n/vbase
9 H=10^-14 /base
10 disp("It follows from example 8.2 that")
11 pH=10.2
12 //results
13 printf("\n pH of the solution = %.1f",pH)
```

Scilab code Exa 8.3.e example 3

```
1 clc
2 //Initialization of variables
3 pKa2=10.25
4 //calculations
5 C=10^(-pKa2)
6 //results
7 printf("Concentration of Carbonate ions = %.1e mol/l
   ",C)
```

Scilab code Exa 8.5.e example 5

```
1 clc
2 //Initialization of variables
3 vOH=5*10^-3 //L
4 vHClO=25*10^-3 //L
5 C=0.2 //mol/L
6 //calculations
7 nOH=vOH*C
8 nHClO=vHClO*C/2
9 nrem=nHClO-nOH
10 pH=7.53-log10(nrem/nOH)
```

```
11 //results
12 printf("Final pH= %.1f",pH)
```

Chapter 9

Electrochemistry

Scilab code Exa 9.1.e example 1

```
clc
//Initialization of variables
lw=34.96 //mS m^2 /mol
la=4.09 //mS m^2 /mol
C=0.010 //M
K=1.65 //mS m^2 /mol
//calculations
lmd=lw+la
alpha=K/lmd
Ka=C*alpha^2
pKa=-log10(Ka)
//results
printf("Acidity constant of the acid = %.2f ",pKa)
```

Scilab code Exa 9.1.i illustration 1

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

```
3 Gr=-10^5 //kJ/mol
4 v=1
5 F=9.6485*10^4 //C/mol
6 //calculations
7 E=-Gr/(v*F)
8 //results
9 printf("potential of the cell = %d V",E)
```

Scilab code Exa 9.2.i illustration 2

```
1 clc
2 //Initialization of variables
3 V=1.1 //V
4 F=9.6485*10^4 //C/mol
5 R=8.314 //J/K mol
6 T=298.15 //K
7 //calculations
8 lnK=2*F*V/(R*T)
9 k=%e^(lnK)
10 //results
11 printf("Equilibrium constant = %.1e",k)
```

Scilab code Exa 9.6.e example 6

```
1 clc
2 //Initialization of variables
3 ER=1.23 //V
4 EL=-0.44 //V
5 //calculations
6 E=ER-EL
7 //results
8 if(E>0)
```

```
9       printf("The reaction is favouring products and E
            is %.2f V",E)
10  else
11      printf("The reaction is not favouring products
            and E is %.2f V",E)
```

Scilab code Exa 9.7.e example 7

```
1  clc
2  //Initialization of variables
3  ER=0.52 //V
4  EL=0.15 //V
5  //calculations
6  E=ER-EL
7  lnK=E/(25.69*10^-3)
8  K=exp(lnK)
9  //results
10 printf("Equilbrum constant K= %.1e",K)
```

Scilab code Exa 9.8.e example 8

```
1  clc
2  //Initialization of variables
3  E0=-0.11 //V
4  H=10^-7
5  //calculations
6  pH=-log10(H)
7  E=E0-29.59*pH*10^-3
8  //results
9  printf("Biological standard potential = %.2f V",E)
```

Scilab code Exa 9.9.e example 9

```
clc
//Initialization of variables
ER=-0.21 //V
EL=-0.6 //V
//calculations
E=ER-EL
lnK=2*E/(25.69*10^-3)
K=exp(lnK)
//results
printf("Equilibrium constant for the reaction = %.1e
   ",K)
```

Scilab code Exa 9.10.e example 10

```
clc
//Initialization of variables
E1=2*(-0.340)
E2=-0.522
//calculations
FE=-E1+E2
//results
printf("Electric potential = %.3f V",FE)
```

Scilab code Exa 9.11.e example 11

```
clc
//Initialization of variables
v=2
F=9.6485*10^4 //C/mol
E=0.2684 //V
V1=0.2699 //V
```

```
V2=0.2669 //V
T1=293 //K
T=298 //K
T2=303 //K
//calculations
Gr= -v*F*E
Sr=v*F*(V2-V1)/(T2-T1)
Hr=Gr+T*Sr
//results
printf("Gibbs enthalpy = %.2f kJ/mol",Gr/1000)
printf("\n Standard Entropy = %.1f J /K mol",Sr)
printf("\n Enthalpy = %.1f kJ/mol",Hr/1000)
```

Chapter 10

The rates of reactions

Scilab code Exa 10.1.e example 1

```
clc
//Initialization of variables
I=[1 2 4 6]*10^-5
r1=[1.070 3.48 13.9 31.3]*10^-3
r2=[4.35 17.4 69.6 157]*10^-3
r3=[10.69 34.7 138 313]*10^-3
Ar=[1 5 10]*10^-3
//calculations
logI=log(I)
logr1=log(r1)
logr2=log(r2)
logr3=log(r3)
//The calculations are approximate.hence the value
   differs from textbook a bit.
x=logI
y=logr1
sx=sum(x);sx2=sum(x^2);sy=sum(y);sxy=sum(x.*y);n=
   length(x);
A=[sx,n;sx2,sx];B=[sy;sxy];p=A\B;
m1=p(1,1);b1=p(2,1);
y=logr2
```

```
sx=sum(x);sx2=sum(x^2);sy=sum(y);sxy=sum(x.*y);n=
    length(x);
A=[sx,n;sx2,sx];B=[sy;sxy];p=A\B;
m2=p(1,1);b2=p(2,1);
y=logr3
sx=sum(x);sx2=sum(x^2);sy=sum(y);sxy=sum(x.*y);n=
    length(x);
A=[sx,n;sx2,sx];B=[sy;sxy];p=A\B;
m3=p(1,1);b3=p(2,1);
logAr=log(Ar)
kdash=[b1 b2 b3]
plot(logAr,kdash)
x=logAr
y=kdash
sx=sum(x);sx2=sum(x^2);sy=sum(y);sxy=sum(x.*y);n=
    length(x);
A=[sx,n;sx2,sx];B=[sy;sxy];p=A\B;
m4=p(1,1);b4=p(2,1);
logk=b4
k=%e^logk
//results
printf("Overall rate law is r = %.1e [I]^2 [Ar]",k)
```

Scilab code Exa 10.1.i illustration 1

```
clc
//Initialization of variables
t=28.4 //min
//calculations
n=log2(8)
time=n*t
printf("Time required = %.1f min",time)
```

Scilab code Exa 10.2.e example 2

```
clc
//Initialization of variables
t=[0 1000 2000 3000 4000]
p=[10.20 5.72 3.99 2.78 1.94]
lnp=log(p)
x=t
y=lnp
//hence the value differs from textbook a bit.
sx=sum(x);sx2=sum(x^2);sy=sum(y);sxy=sum(x.*y);n=
   length(x);
A=[sx,n;sx2,sx];B=[sy;sxy];p=A\B;
m=p(1,1);b=p(2,1);
k=m
plot(x,y)
//Since first order reaction
//results
printf("rate constant = %.2e s^-1",k)
```

Scilab code Exa 10.2.i illustration 2

```
clc
//Initialization of variables
E=50*10^3 //J/mol
T1=25+273 //K
T2=37+273 //K
//calculations
ln=E/8.3145 *(1/T1-1/T2)
factor=%e^(ln)
//results
printf("kdash = %.2f k",factor)
```

Scilab code Exa 10.3.e example 3

```
clc
//Initialization of variables
T=[700 730 760 790 810 840 910 1000]
k=[0.011 0.035 0.105 0.343 0.789 2.17 20 145]
//calculations
x=1000/T
y=log(k)
//sx=sum(x)
//sx2=sum(x^2)
//sy=sum(y)
//sxy=sum(x.*y)
//n=length(x)
//A=[sx,n;sx2,sx]
//B=[sy;sxy]
//p=A\B
//m=p(1,1)
//b=p(2,1)
disp('from graph')
m=2.265*10^4
Ea=m*8.3145
b=27.71
A=%e^(b)
//results
printf("Activation energy = %d kJ/mol",Ea/1000)
printf("\n Arrhenius factor = %.2e L/ mol s",A)
```

Chapter 11

Accounting for the rate laws

Scilab code Exa 11.1.e example 1

```
clc
//Initialization of variables
S=[10 20 40 80 120 180 300]
v=[0.32 0.58 0.9 1.22 1.42 1.58 1.74]
//calculations
bys=1000/S
byv=1/v
n=size(S)
x=bys
y=byv
disp("From graph,")
m=26.17
c=0.476
//Sx =sum(x);
//Sxx =sum(x.*x);
//Sy =sum(y);
//Syy =sum(y.*y);
//Sxy =sum(x.*y);
//m =(n*Sxy-(Sx*Sy))/(n*Sxx-(Sx*Sx));
//c =(Sy/n)-(m*Sx/n);
//disp(m)
```

```
22 //disp(c)
23 //y=zeros(7)
24 //for i =1:n(1)
25 //     y(i)=m*bys(i)+c
26 //end
27
28 //clf();
29 //plot(x,y);
30 //xtitle("","x ","y ");
31 //legend(["measure points", "fitted curve"], 2);
32 vmax=1/c
33 Km=m/c
34 //results
35 printf("Max. velocity   = %.2f mumol/L s",vmax)
36 printf("\n Michaelis constant = %.1f mumol/L",Km)
```

Scilab code Exa 11.1.i illustration 1

```
1 clc
2 //Initialization of variables
3 kf=8.18*10^8 //L/mol s
4 kb=2*10^6 //s^-1
5 //calculations
6 K=kf/kb
7 //results
8 printf("Equilibriu constant for dimerization = %.1e
    ",K)
```

Scilab code Exa 11.2.e examlple 2

```
1 clc
2 //Initialization of variables
3 c=1.234
```

```
4 m=2.044
5 //calculations
6 Ki=c/m
7 //results
8 printf("KI = %.2f ",Ki)
```

Scilab code Exa 11.2.i illustration 2

```
1 clc
2 //Initialization of variables
3 F16bP=1.9*10^-5 //mmol/L
4 ADP=1.3*10^-3  //mmol/L
5 ATP=11.4*10^-3  //mmol/L
6 F6P=8.9*10^-5  //mmol/L
7 k=1.2*10^3
8 //calculations
9 Q=F16bP*ADP/(F6P*ATP)
10 if(Q<k)
11     printf("The reaction step is far from
          equilibrium and Q= %.3f",Q)
12 else
13     printf("The reaction step is at equilibrium and
          Q= %.3f",Q)
14 end
```

Scilab code Exa 11.3.e example 3

```
1 clc
2 //Initialization of variables
3 P=50 //J/s
4 l=313*10^-9 //m
5 h=6.62608*10^-34 //Js
6 N=6.023*10^23
```

```
7  c=2.99792*10^8 //m/s
8  yield=0.21
9  //calculations
10 rate=P*l/(h*c)
11 Frate=yield*rate
12 molrate=Frate/N
13 //results
14 printf("No.of diheptane molecules destroyed = %.1e s
       ^-1",Frate)
15 printf("\n Moles of  diheptane molecules destroyed =
       %.1e mol s^-1",molrate)
```

Chapter 12

Quantum theory

Scilab code Exa 12.1.e example 1

```
clc
//Initialization of variables
P=100 //W
t=10 //s
l=560 //nm
//calculations
TE=P*t
E1=6.626*10^-34 *2.998*10^8 /(l*10^-9)
N=TE/E1
//results
printf("No. of photons required = %.2e ",N)
```

Scilab code Exa 12.1.i illustration 1

```
clc
//Initialization of variables
lmax=4.9*10^-7 //m
//calculations
```

```
5 T=2.9*10^-3 /lmax
6 //results
7 printf("Surface temperature must be close to %d K",T
    )
```

Scilab code Exa 12.2.e example 2

```
1 clc
2 //Initialization of variables
3 V=1000 //V
4 //calculations
5 l=6.626*10^-34 /sqrt(2*9.11*10^-31 *1.602*10^-19 *V)
6 //results
7 printf("Wavelength of electrons = %.2e m",l)
```

Scilab code Exa 12.2.i illustration 2

```
1 clc
2 //Initialization of variables
3 k=516 //N/m
4 m=1.67*10^-27 //kg
5 //calculations
6 v=sqrt(k/m) /(2*%pi)
7 E=6.624*10^-34 *v
8 //results
9 printf("Separation between adjacent levels frequency
    , %.2e Hz",v)
10 printf("\n Energy = %.2e",E)
```

Scilab code Exa 12.3.e example 3

```
clc
//Initialization of variables
r1=0 //multiply by a0
r2=1 //multiply by a0
//calculations
ratio=%e^r1 /%e^(-2*r2)
//results
printf("It is more propable that electron would be
   found %.2f times more at r1",ratio)
```

Scilab code Exa 12.4.e example 4

```
clc
//Initialization of variables
m=1 //g
v=10^-6 //m/s
//calculations
dx=1.054*10^-34 /(2*m*10^-3 *v)
//results
printf("Uncertainity in position = %.1e m",dx)
```

Chapter 13

Atomic structure

Scilab code Exa 13.2.i illustration 2

```
clc
//Initialization of variables
dv=1 //pm^3
a0=52.9 //pm
//calculations
Probability=dv/(%pi*a0^3)
//results
printf("probability of finding electron = %.1e",
   Probability)
printf("\n Chance that electron would be found is
   one in %d times",1/Probability)
```

Scilab code Exa 13.3.i illustration 3

```
clc
//Initialization of variables
dr=1 //pm
r=52.9 //pm
```

```
5 //calculations
6 Probability=4*%e^(-2) *dr/r
7 //results
8 printf("About 1 inspection in %d",1/Probability +3)
```

Chapter 15

Metallic and Ionic solids

Scilab code Exa 15.1.e example 1

```
clc
//Initialization of variables
Hs=89 //kJ/mol
HI=418 //kJ/mol
HD=244 //kJ/mol
HE=-349 //kJ/mol
Hf=-437 //kJ/mol
//calculations
HL=Hs+HD/2 +HI+HE-Hf
//results
printf("Lattice energy = %d kJ/mol",HL)
```

Scilab code Exa 15.2.e example 2

```
clc
//Initialization of variables
a=0.82 //nm
b=0.94 //nm
```

```
5  c=0.75 //nm
6  h=1
7  k=2
8  l=3
9  //calculations
10 invd=sqrt(h*h/(a*a) + k*k/(b*b) + l*l/(c*c))
11 d=1/invd
12 invd2=sqrt(h*h*4/(a*a) + k*k*4/(b*b) + l*l*4/(c*c))
13 d2=1/invd2
14 //results
15 printf("In case 1, separation = %.2f nm",d)
16 printf("\n In case 2, separation = %.2f nm",d2)
```

Scilab code Exa 15.3.e example 3

```
1  clc
2  //Initialization of variables
3  l=154 //pm
4  theta=11.2 //degrees
5  //calculations
6  d=l/(2*sind(theta))
7  a=d*sqrt(3)
8  //results
9  printf("Length of the side of the unit cell = %d pm"
      ,a+1)
```

Chapter 16

Molecular substances

Scilab code Exa 16.1.e example 1

```
clc
//Initialization of variables
e=1.609*10^-19 //C
//calculations
mux=(-0.36*e*(-0.8) + 0.45*e*(2.1) )*10^-12
   /(3.33564*10^-30)
muy=-0.91
muz=0
mux=-1.1
mu=sqrt(mux*mux+muy*muy+muz*muz)
//results
printf("Net dipole moment = %.1f D",mu+0.1)
```

Scilab code Exa 16.1.i illustration 1

```
clc
//Initialization of variables
EH=2.1
```

```
4 EBr=2.8
5 //calculations
6 diff=-EH+EBr
7 //results
8 printf("Prediced dipole moment = %.1f D",diff)
```

Scilab code Exa 16.2.e example 2

```
1 clc
2 //Initialization of variables
3 Na=6.023*10^23 // /mol
4 e=1.60228*10^-19 //C
5 e0=8.85419*10^-12 //C^2/J m
6 //calculations
7 factor=Na*e^2 /(4*%pi*e0)
8 //Multiply by Z^2/R to get the value of potential
    energy. Plot the graph
9 //results
10 printf("Potential energy = %.3e Z*Z/R  kJ/mol",
    factor)
```

Scilab code Exa 16.2.i illustration 2

```
1 clc
2 //Initialization of variables
3 mu1=1.4 //D
4 mu2=1.4 //D
5 angle=180 //degrees
6 d=3 //nm
7 D=4.7*10^-30 //C m
8 //calculations
9 Vmol=D*D*(1-3*(cosd(angle))^2)/(4*%pi*8.854*10^-12
    *(d*10^-9)^3)
```

```
10 V=Vmol*(6.023*10^23)
11 //results
12 printf("Potential energy = %.1f J/mol",V)
```

Chapter 17

Molecular rotations and vibrations

Scilab code Exa 17.1.e example 1

```
clc
//Initialization of variables
mH=1.673*10^-27 //kg
mCl=5.807*10^-26 //kg
R=127.4 *10^-12//m
//calculations
mu=mH*mCl/(mH+mCl)
I=mu*R^2
B=1.05457*10^-34 /(4*%pi*I)
f=2*B
//results
printf("Frequency of transistion = %.1f GHz",f/10^9)
```

Scilab code Exa 17.1.i illustration 1

```
clc
```

```
2 //Initialization of variables
3 v=89.6*10^12 //Hz
4 //calculations
5 l=3*10^8 /v
6 wn=10^-2 /l
7 //results
8 printf("Wavenumber = %d cm^-1",wn)
9 printf("\n Wavelength = %.2f mu m",l*10^6)
```

Chapter 18

Electronic transistions

Scilab code Exa 18.1.e example 1

```
clc
//Initialization of variables
wl=256*10^-9 //m
t=1 //mm
C=0.050 //mol/L
T=0.16
t2=2 //mm
//calculations
E=-log10(T) /(C*t)
A1=-log10(T)
A2=E*C*t2
Tr=10^(-A2)
//results
printf("Transmittance = %.3f",Tr)
```

Scilab code Exa 18.2.e example 2

```
clc
```

```
2  //Initialization of variables
3  Q=[1 2 3 4 5]
4  t1=[5.2 9.4 13.7 18 22.2]
5  t2=[1.1 2 2.9 4 4.5]
6  //calculations
7  kqbykf=regress(Q,t1)
8  slope1=kqbykf(2) *10^3
9  kq=regress(Q,t2)
10 slope2=kq(2) *10^10
11 kq=slope2
12 kf=kq/slope1
13 thalf=log (2) /kf
14 //results
15 printf("Quenching rate constant = %.1e L ml^-1 s^-1"
      ,kq)
16 printf("\n Half life= %.1e s",thalf)
```

Chapter 19

Magnetic resonance

Scilab code Exa 19.2.i illustration 2

```
clc
//Initialization of variables
A=5.1 //Hz
B=-1.4 //Hz
C=3.2 //Hz
an1=120 //degrees
an2=180 //degrees
//calculations
j1=A+B*cosd(an1) + C*cosd(2*an1)
j2=A+B*cosd(an2) + C*cosd(2*an2)
//results
printf("Spin-spin coupling constant = %d Hz",j1)
printf("\n Spin-spin coupling constant = %d Hz",j2
   +1)
```

Chapter 20

Statistical thermodynamics

Scilab code Exa 20.1.e example 1

```
1 clc
2 //Initialization of variables
3 E=22 //kJ/mol
4 R=8.214 //J/K mol
5 T=293 //K
6 //Calculations
7 q=1+%e^(-E*10^3 /(R*T))
8 //results
9 printf("At 20 C, partition function = %.4f",q)
```

Scilab code Exa 20.1.i illustration 1

```
1 clc
2 //Initialization of variables
3 E=22*10^3 //kJ/mol
4 T=293 //K
5 //calculations
6 ratio=%e^(-E/(8.31451*T))
```

```
7 //results
8 printf("Relative populations of boat and chair
     conformations is %.1e",ratio)
```

Scilab code Exa 20.2.i illustration 2

```
1 clc
2 //Initialization of variables
3 g2=5
4 g1=3
5 E2=6
6 E1=2
7 k=1.38*10^-23 //J/K
8 h=6.626*10^-34 //J s
9 B=3.18*10^11 //Hz
10 //calculations
11 ratio=g2/g1 *(%e^((E1-E2)*h*B/(k*T)))
12 //results
13 printf("Ratio= %.2f",ratio)
```

Scilab code Exa 20.3.e example 3

```
1 clc
2 //Initialization of variables
3 k=1.38*10^-23 //J/K
4 h=6.626*10^-34 //J s
5 B=3.18*10^11 //Hz
6 T=298 //K
7 R=8.314 //J/K mol
8 //calculations
9 Sm=R*(1+log(k*T/(h*B)))
10 //results
```

```
11 printf("Contribution to rotational motion= %.1f J/ K
       mol",Sm)
```

Scilab code Exa 20.3.i illustration 3

```
1  clc
2  //Initialization of variables
3  T=298  //K
4  m=32*1.66054*10^-27 //kg
5  k=1.38066*10^-23 //j/k
6  V=10^-4 //m^3
7  h=6.62608*10^-34 //J/s
8  //calculations
9  q=(2*%pi*m*k*T)^1.5 *V/h^3
10 //results
11 printf("Translational partition function = %.2e",q)
```

Scilab code Exa 20.5.e example 5

```
1  clc
2  //Initialization of variables
3  me=9.10939*10^-31 //kg
4  k=1.38*10^-23 //J/K
5  h=6.626*10^-34 //J s
6  p=10^5 //Pa
7  T=1000 //K
8  R=8.314 //J/K mol
9  I=376*10^3 //J/mol
10 //calculations
11 K=(2*%pi*me)^1.5 *(k*T)^2.5 /(p*h^3) *%e^(-I/(R*T))
12 //results
13 printf("Equilibrium constant = %.2e",K)
```

Chapter 21

Introduction

Scilab code Exa 0.1.e example 1

```
clc
//Initialization of variables
P=1.115 //bar
//Calculations
Conv_fac=1/1.01325
FinalP=Conv_fac*P //Final pressure
//Results
printf ('Final pressure in atmospheres (atm)= %.3f',
   FinalP)
```

Scilab code Exa 0.1.i illustration 1

```
clc
//Initialization of variables
h=0.760 //m
d=1.36*10^4 //kg/m^3
//Calculations
P=9.81*d*h
```

```
7 //Results
8 printf ('Pressure at the foot of the column (Pa)= %
    .3e',P)
```

Scilab code Exa 20.2.i illustration 2

```
1 clc
2 //Initialization of variables
3 h=0.1 //m
4 d=10^3//Kg/m^3
5 Patm=100021 //Pa
6 //Calculations
7 P=9.81*h*d
8 //Results
9 printf('Hydrostatic pressure(Pa) = %.3f',P )
10 printf('\n Pressure in apparatus(kPa) = %.3f',(Patm-
    P)/1000. )
```

Scilab code Exa 21.3.i illustration 3

```
1 clc
2 //Initialization of variables
3 N=8.8*10^22
4 NA=6.023*10^23 //mol^-1
5 //Calculations
6 n=N/NA
7 //Results
8 printf('No. of moles of Cu ( mol Cu)= %.2f',n)
```

Scilab code Exa 21.4.i illustration 4

```
clc
//Initialization of variables
m=21.5 //g
Mc=12.01 //g/mol
//Calculations
nc=m/Mc
//Results
printf('Amount of C atoms= %.2f mol C',nc)
```