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
```

```
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
```

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

Scilab code Exa 3.2.e example 2

```
clc
//Initialization of variables
m=1 //g
MW=24.31 //g/mol
H=2337 //kJ/mol
//Calculations
n=m/MW
q=n*H
//results
printf('Heat supplied = %.1f kJ',q)
```

Scilab code Exa 3.3.e example 3

```
clc
//Initialization of variables
HC=716.68 //kJ
HH=871.88 //kJ
HO=249.17 //kJ
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

```
clc
//Initialization of variables
Power=100 //W
time=1 //day
T=20 //C
//calculations
timeins=1*24*3600
qsurr=timeins*Power
Ssurr=qsurr/(T+273)
//results
printf('Heat transferred to surroundings = %d J',
   qsurr)
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
```

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

Scilab code Exa 4.3.i illustration 3

```
clc
//Initialization of variables
SH2O=70 //J/K mol
SH2=131 //J/K mol
SO2=205 //J/K mol
//calculations
deltaS=2*SH2O-2*SH2-SO2
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
```

```
mW=50 //g
//calculations
nE=mE/46
nW=mW/18
ntotal=nE+nW
xE=nE/ntotal
xW=1-xE
disp('for the observed xE and xW')
vE=55 //cc/mol
vW=18 //cc/mol
V=nE*vE+nW*vW
//results
printf('\n VOlume of the mixture = %d cm^3 ',V+1)
```

Scilab code Exa 6.3.e example 3

```
clc
//Initialization of variables
xc=[0 0.20 0.40 0.60 0.80 1]
pc=[0 35 82 142 219 293]
pa=[347 270 185 102 37 0]
//calculations
plot(xc,pc)
plot(xc,pa)
xlabel('Mole fraction xc')
ytitle('Pressure /Torr')
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

```
clc
```

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

Scilab code Exa 6.5.e example 5

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

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

Scilab code Exa 6.6.e example 6

```
clc
//Initialization of variables
nB=0.59 //mol
nNB=0.41 //mol
xN1=0.38
xN2=0.74
xNm=0.41
//calculations
disp('By lever rule')
ratio=(xNm-xN1)/(xN2-xNm)
percent=ratio*100
//results
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
```

```
PH2=3-3*sol
PNH3=2*sol
K=PNH3^2/(PH2^3 *PN2)
//results
printf("Pressure of N2 gas =%.2f bar",PN2)
printf("\n Pressure of H2 gas =%.2f bar",PH2)
printf("\n Pressure of NH3 gas =%.2f bar",PNH3)
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
```

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

Scilab code Exa 8.3.e example 3

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

Scilab code Exa 8.5.e example 5

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

```
//results
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
```

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

Scilab code Exa 9.2.i illustration 2

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

Scilab code Exa 9.6.e example 6

```
clc
//Initialization of variables
ER=1.23 //V
EL=-0.44 //V
//calculations
E=ER-EL
//results
if(E>0)
```

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

Scilab code Exa 9.7.e example 7

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

Scilab code Exa 9.8.e example 8

```
clc
//Initialization of variables
E0=-0.11 //V
H=10^-7
//calculations
pH=-log10(H)
E=E0-29.59*pH*10^-3
//results
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)
```

```
//disp(c)
//y=zeros(7)
//for i =1:n(1)
//     y(i)=m*bys(i)+c
//end

//clf();
//plot(x,y);
//xtitle("","x ","y ");
//legend([" measure points", "fitted curve"], 2);
vmax=1/c
Km=m/c
//results
printf("Max. velocity  = %.2f mumol/L s",vmax)
printf("\n Michaelis constant = %.1f mumol/L",Km)
```

Scilab code Exa 11.1.i illustration 1

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

Scilab code Exa 11.2.e examlple 2

```
clc
//Initialization of variables
c=1.234
```

```
m=2.044
//calculations
Ki=c/m
//results
printf("KI = %.2f ",Ki)
```

Scilab code Exa 11.2.i illustration 2

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

Scilab code Exa 11.3.e example 3

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

```
c=2.99792*10^8 //m/s
yield=0.21
//calculations
rate=P*l/(h*c)
Frate=yield*rate
molrate=Frate/N
//results
printf("No.of diheptane molecules destroyed = %.1e s
    ^-1",Frate)
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
```

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

Scilab code Exa 12.2.e example 2

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

Scilab code Exa 12.2.i illustration 2

```
clc
//Initialization of variables
k=516 //N/m
m=1.67*10^-27 //kg
//calculations
v=sqrt(k/m) /(2*%pi)
E=6.624*10^-34 *v
//results
printf("Separation between adjacent levels frequency
   , %.2e Hz",v)
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
```

```
//calculations
Probability=4*%e^(-2) *dr/r
//results
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
```

```
c=0.75 //nm
h=1
k=2
l=3
//calculations
invd=sqrt(h*h/(a*a) + k*k/(b*b) + l*l/(c*c))
d=1/invd
invd2=sqrt(h*h*4/(a*a) + k*k*4/(b*b) + l*l*4/(c*c))
d2=1/invd2
//results
printf("In case 1, separation = %.2f nm",d)
printf("\n In case 2, separation = %.2f nm",d2)
```

Scilab code Exa 15.3.e example 3

```
clc
//Initialization of variables
l=154 //pm
theta=11.2 //degrees
//calculations
d=l/(2*sind(theta))
a=d*sqrt(3)
//results
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
```

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

Scilab code Exa 16.2.e example 2

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

Scilab code Exa 16.2.i illustration 2

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

```
V=Vmol*(6.023*10^23)
//results
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
```

```
//Initialization of variables
v=89.6*10^12 //Hz
//calculations
l=3*10^8 /v
wn=10^-2 /l
//results
printf("Wavenumber = %d cm^-1",wn)
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
```

```
//Initialization of variables
Q=[1 2 3 4 5]
t1=[5.2 9.4 13.7 18 22.2]
t2=[1.1 2 2.9 4 4.5]
//calculations
kqbykf=regress(Q,t1)
slope1=kqbykf(2) *10^3
kq=regress(Q,t2)
slope2=kq(2) *10^10
kq=slope2
kf=kq/slope1
thalf=log (2) /kf
//results
printf("Quenching rate constant = %.1e L ml^-1 s^-1"
   ,kq)
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

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

Scilab code Exa 20.1.i illustration 1

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

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

Scilab code Exa 20.2.i illustration 2

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

Scilab code Exa 20.3.e example 3

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

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

Scilab code Exa 20.3.i illustration 3

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

Scilab code Exa 20.5.e example 5

```
clc
//Initialization of variables
me=9.10939*10^-31 //kg
k=1.38*10^-23 //J/K
h=6.626*10^-34 //J s
p=10^5 //Pa
T=1000 //K
R=8.314 //J/K mol
I=376*10^3 //J/mol
//calculations
K=(2*%pi*me)^1.5 *(k*T)^2.5 /(p*h^3) *%e^(-I/(R*T))
//results
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
```

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

Scilab code Exa 20.2.i illustration 2

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

Scilab code Exa 21.3.i illustration 3

```
clc
//Initialization of variables
N=8.8*10^22
NA=6.023*10^23 //mol^-1
//Calculations
n=N/NA
//Results
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)
```