Scilab Textbook Companion for Chemistry In Engineering And Technology Volume 1 by J. C. Kuriacose And J. Rajaram[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 1

Atomic Structure

Scilab code Exa 1.1 Relative Abundance

```
1 printf('The Atomic weight of 12.0111 for Natural
    Carbon shows that the 12C nuclide must be present
     to a larger extent.');
2 printf('\nLet 100 atoms of natural carbon contain x
    atoms of 12C nuclide.\n');
3 X=(13.0034-12.0111)*100/(13.0034-12.0000);//
    percentage of 12C in natural carbon//
4 printf('Percentage of 12C in Natural carbon=X=%f',X)
    ;
5 Y=100-X;//percentage of 13C in natural carbon//
6 printf('\nPercentage of 13C in Natural carbon=%f',Y)
    ;
```

Scilab code Exa 1.2 Frequency and Wavenumber

```
1 C=3*10^2;//velocity of light in megametre/sec//
2 L=300*10^-9;//wavelength of radiation in metres//
3 v=C*10^-6/L;//frequency of radiation in Teracycles
    per sec//
```

```
4 printf('Frequency of radiation=v=%fTeracycles per
    sec=1.0*10^15Hz',v);
5 v1=1/L;//wave number of radiation in per meter//
6 printf('\nWavenumber of radiation=v1=3.3*10^4 per
    centimeter');
```

Scilab code Exa 1.3 Velocity of photoelectrons

```
1 V=0.85;//external voltage in volts//
2 e=1.6*10^-19;//electron charge in coloumbs//
3 m=9.1*10^-28;//electron mass in grams//
4 v=sqrt(2*V*e*10/m);//velocity of electron in motion
    in Kilocm per sec//
5 printf('velocity of electron in motion=v=%f Kilocm
    per sec=5.47*10^7cm per sec',v);
6 W=(3.198*10^-12)/(1.6*10^-12);//Threshold energy in
    eV//
7 printf('\nThreshold energy of electron=W=%feV',W);
8 v0=(3.198*10^-12)/(6.625*10^-15);//Threshold
    frequency in tera per sec//
9 printf('\nThreshold frequency=v0=%fTera per sec
    =4.83*10^14per sec',v0);
```

Scilab code Exa 1.4 Wavelength

```
1 E=118.5*10^3*4.2*10^7;//energy of ions in ergs//
2 C=3*10^10;//velocity of light in cm/sec//
3 L=6.023*10^23;//Avagadro number//
4 h=6.625*10^-27;//plank's constant//
5 l=(L*h*C*10^8)/E;
6 printf('wavelength required to cause ionization=l=
    %fAngstrums',l);
```

Scilab code Exa 1.5 Wavelength of the second line

```
n1=2;
n2=4;
dE=21.7*(10^-12)*((1/n1^2)-(1/n2^2));
h=6.625*10^-27;//plank's constant//
C=3*10^10;//velocity of light in cm/sec//
l=h*C*10^8/dE;//Wavelength of second line in balmer
   series in Angstrums//
printf('wavelength of the second line in balmer
   series=l=%fAngstrums',l);//here the answer given
   in textbook is slightly wrong the original answer
    should be the one comes through execution//
```

Scilab code Exa 1.6 Ionization potential

```
n1=1;
dE=21.7*(10^-12)/(1.6*10^-12*n1^2);//energy required
    to promote an electron from ground to infinity
   in eV//
printf('Ionisation potential for an electron=dE=%feV
   ',dE);
```

Scilab code Exa 1.7 De Broglie Wavelength

```
h=6.625*10^-27;//plank's constant//
V=2*10^3;//velocity of Cricket Ball in cm/sec//
m=170;//weight of Cricket Ball in grams//
l=h/(m*V);//DeBroglie Wavelength of CricketBall in
   Angstrums//
```

```
5 printf('DeBroglie Wavelength of CricketBall=l=%f
    =1.95*10^-24Angstrums',l);
```

Scilab code Exa 1.8 De Broglie Wavelength

```
1 r1=0.53*10^-8;//Bohr radius in cm//
2 r2=4*r1;//Bohr radius in second state in cm//
3 printf('Bohr radius in second state=r2=2.12*10^-8cm'
    );
4 h=6.625*10^-27;//plank's constant//
5 m=9.11*10^-28;//electron mass in grams//
6 v2=h/(%pi*m*r2);//electron velocity in second state
    in cm per sec//
7 printf('\nElectron velocity in second state=v2=%fcm
    per sec',v2);
8 l=(h*10^8)/(m*v2);//De Broglie wavelength of
    electron in second state in Angstrums//
9 printf('\nDe Broglie wavelength of electron in
    second state=l=%fAngstrums',l);
10 e=1.6*10^-12;//electron charge in ergs//
11 v=sqrt((2*(10^4)*e)/m);//velocity of the moving
    electron in second state in cm/sec//
12 printf('\nVelocity of moving electron in second
    state=v=%fcm per sec',v);
13 l1=(h*10^8)/(v*m);//De Broglie wavelength of moving
    elctron in Angstrums//
14 printf('\nDe Broglie wavelength of moving electron
    in secondstate=l1=%fAngstrums',l1);
```

Scilab code Exa 1.9 Uncertainity in position

```
1 m=9.11*10^-28;//electron mass in grams//
2 v=1.1*10^8;//velocity of electron in cm per sec//
```

```
3 p=m*v;//momentum of electron in gram cm per sec//
4 printf('momentum of electron=p=10.01*10^-20gram cm
    per sec');
5 dp=p*10^-2;//Uncertainity in momentum in gram cm per
    sec//
6 printf('\nUncertainity in momentum=10.01*10^-22gram
    cm per sec');
7 h=6.625*10^-27;//plank's constant//
8 dx=(h*10^8)/(4*%pi*dp);//Uncertainity in position in
    Angstrum//
9 printf('\nUncertainity in position=dx=%fAngstrum',dx
    );
```

Scilab code Exa 1.10 Energy difference between energy levels

```
1 h=6.625*10^-27;//plank's constant//
2 g=10^3;//particle mass in grams//
3 l1=1;//length of one dimensional box in cm//
4 n1=1;
5 n2=2;
6 dE1=((n2^2-n1^2)*h^2)/(8*g*l1^2);//Energy difference
    between two energy levels of particle in eV//
7 printf('Energy difference between two energy levels
    of particle=dE1=1*10^-44eV');
8 l2=2*10^-8;//length of one dimensional box in cm//
9 m=9.11*10^-28;//electron mass in grams//
10 dE2=((n2^2-n1^2)*h^2)/(8*m*l2^2*1.6*10^-11);//Energy
    difference between two energy levels of electron
    in eV//
11 printf('\nEnergy difference between two energy
    levels of electron=dE2=%feV',dE2);
```

Chapter 2

Nuclear Structure and Radioactivity

Scilab code Exa 2.1 Half life of a radioactive nuclide

```
1 N0=3396;//no. of counts per minute given by
    radioactive nuclide at a given time//
2 N=1000;//no. of counts per minute given by
    radioactive nuclide one hour later//
3 thalf=0.693*60/(2.303*log(N0/N));//half life of
    nuclide in minutes//
4 printf('Half life of radioactive nuclide=t1/2=
    %fminutes',thalf);
5 t1=2.303*log(100/25)*thalf/0.693;//time required for
     the activity to decrease to 25% of the initial
    activity in minutes//
6 printf('\nTime required for the activity to decrease
     to 25percent of the initial activity=t1=
    %fminutes',t1);
7 t2=2.303*log(100/10)*thalf/0.693;//time required for
     the activity to decrease to 10% of the initial
    activity in minutes//
8 printf('\nTime required for the activity to decrease
     to 10percent of the initial activity=t2=
```

```
%fminutes',t2);
```

Scilab code Exa 2.2 Half life of a radioactive nuclide

```
R=3.7*10^10;//no. of alpha particles per second
   emitted by 1g of 226Ra//
N=(6.023*10^23)/226;//no. of atoms of 226Ra//
yr=3.15*10^7;//no of seconds in a year//
thalf=0.693*N/(R*yr);//half life of 226Ra in years//
printf('Half life of 226Ra molecule=t1/2=%fyears',
   thalf);//here the answer written in textbook is
   wrongly printed actual answer will be the one we
   are getting here//
```

Scilab code Exa 2.3 Weight of 1Ci

```
thalf=14.8*60*60;//half life of 24Na atom in seconds
   //
L=6.023*10^23;//Avagadro number//
v=3.7*10^10;//1 Ci of radioactivity in
   disintegrations per second//
w=(24*10^6*v*thalf)/(0.693*L);//weight of 1 Ci of 24
   Na in grams//
printf('Weight of 1 Ci of 24Na=w=%fmicrograms
   =1.13*10^-7grams',w);
```

Scilab code Exa 2.4 Binding Energy

```
Mp=1.00728;//mass of proton in amu//
Mn=1.00866;//mass of neutronin amu//
```

```
3 MH=2.01355;//isotopic mass of H atom in amu//
4 dM=((1*Mp)+(1*Mn)-MH);//dM value of H atom in amu//
5 printf('dM value of H atom=dM=%famu',dM);
6 BE=dM*931;//binding energy of H atom in MeV//
7 printf('\nBinding energy of H atom=BE=%fMeV',BE);
```

Scilab code Exa 2.5 Age of a Specimen

```
1 N0=15.3;//decay rate of Contemporary Carbon in
    disintegrations/min/gram//
2 N=2.25;//decay rate of 14C specimen in
    disintegrtions/min/gram//
3 thalf=5670;//half life of nuclide in years//
4 t=2.303*log(N0/N)*thalf/0.693;//Age of the specimen
    in years//
5 printf('Age of the specimen=t=%fyears',t);//here the
     answer given in textbook is actually wrong we
    get twice that of the answer which is shown
    through execution//
```

Scilab code Exa 2.6 Age of a Specimen

```
1 thalf=4.5*10^9;//half life of Uranium in years//
2 printf('Here N0 and N must be in terms of Uranium.N
    is proportional to 1gram og Uranium');
3 printf('\nN0 can be calculated from the given data
    .0.0453grams of 206Pb corresponds to
    238*0.0453/206=0.0523grams of 238U,i.e 0.0453
    grams of 206Pb must have been formed by the
    decaying of 0.523grams of 238U.\nSince N is
    proportional to 1,N0 is proportional to 1.0523.')
    ;
4 N0=1.0523;
```

```
5 N=1;
6 t=2.303*log(N0/N)*thalf/0.693;//Age of the mineral
    in years//
7 printf('\nAge of the mineral=t=%fyears=7.62*10^8
    years',t);//here also the answer given in
    textbook is wrong the one resulted through
    execution is the right one//
```

Chapter 4

States of matter

Scilab code Exa 4.1 Pressure and Volume of gas

```
1 P=760;//pressure of 14g of nitrogen in mm of Hg//
2 V=22.4;//Volume occupied by 14g of Nitrogen in
    litres//
3 P1=380;//changed pressure of 14g of nitrogen in mm
    of Hg//
4 V1=(P*V)/P1;//changed volume of 14g of nitrogen at
    380mm pressure in litres//
5 printf('Volume of 14g of Nitrogen at 380 mm Hg
    pressure=V1=%flitres',V1);
6 V2=5.6;//changed volume of 14g of nitrogen in litres
    //
7 P2=(P*V)/V2;//Pressure of 14g of nitrogen of volume
    5.6 litres//
8 printf('\nPressure of 14g of Nitrogen of volume 5.6
    litres=P2=%fmm Hg',P2);
```

Scilab code Exa 4.2 Volume and temperature of gas

```
V=5.6;//Volume occupied by 8g of Oxygen at 0 C in
    litres//
T=273;//Temperature at which 8g of Oxygen occupies
    5.6litres in Kelvin//
V1=11.2;//Changed volume of 8g of Oxygen in litres//
T1=(V1*T)/V;//Temperature at which 8g of Oxygen
    occupies 11.6litres in kelvin//
printf('Temperature of 8g of Oxygen Occupying 11.6
    litres=T1=%fKelvin=273degrees',T1);
```

Scilab code Exa 4.3 Volume and temperature of gas

```
P=380;//pressure of 11g of CO2 at 273K in mm of Hg//
T=273;//Initial temperature of 11g of CO2 in kelvin
    //
V=11.2;//Volume occupied by 11g of CO2 in litres at
    273K//
P1=760;//changed pressure of 11g of CO2 at 546K in
    mm of Hg//
T1=546;//Final temperature of 11g of CO2 in kelvin//
V1=(P*V*T1)/(T*P1);//changed volume of 11g of CO2 at
    760mm pressure in litres//
printf('Volume of 11g of CO2 at 760 mm Hg pressure
    at 546K=V1=%flitres',V1);
```

Scilab code Exa 4.4 Number of moles

```
P=570/760;//pressure of 10L of H2 at 300K in
    Atmospheres//
T=300;//Temperature of 10L of H2 in kelvin//
V=10;//Volume occupied by H2 at 300K in litres//
R=0.082;//Value of R in litre-atmospheres//
```

```
5 n=(P*V)/(R*T);//Number of moles of hydrogen present
    //
6 printf('Number of moles of Hydrogen present=n=%fmol'
    ,n);
```

Scilab code Exa 4.5 Volume of dry gas

```
1 TP=746;//Total pressure of gas at 298K in mm of Hg//
2 PP=24;//Partial pressure of Water vapour at 298K in
    mm of Hg//
3 PPG=TP-PP;//partial pressure of gas at 298K in mm of
     Hg//
4 printf('partial pressure of dry gas at 298k=%fmm of
    Hg',PPG);
5 V=200;//Volume occupied by gas at 298K in
    millilitres//
6 P1=760;
7 V1=(PPG*V)/P1;//Volume of dry gas at a pressure of
    760mm Hg//
8 printf('\nVolume of dry gas at pressure 760mm of Hg=
    V1=%fml',V1);
```

Scilab code Exa 4.6 Partial Pressures of gas

```
1 mA=0.11;//amount of gas A in grams//
2 MWA=44;//Molecular weight of gas A in grams//
3 nA=mA/MWA;//No. of moles of gas A//
4 printf('No. of moles of gas A=nA=%fmol',nA);
5 mB=0.17;//amount of gas B in grams//
6 MWB=34;//Molecular weight of gas B in grams//
7 nB=mB/MWB;//No. of moles of gas B//
8 printf('\nNo. of moles of gas B=nB=%fmol',nB);
9 MFA=nA/(nA+nB);//mole fraction of gas A//
```

```
10 printf('\nmole fraction of gas A=MFA=%f',MFA);
11 MFB=nB/(nA+nB);//mole fraction of gas B//
12 printf('\nmole fraction of gas B=MFB=%f',MFB);
13 PPA=MFA*759;//Partial pressure of gas A//
14 printf('\nPartial pressure of gas A=PPA=%fmm of Hg',
     PPA);
15 PPB=MFB*759;//Partial pressure of gas B//
16 printf('\nPartial pressure of gas B=PPB=%fmm of Hg',
     PPB);
```

Scilab code Exa 4.7 Total pressure of mixture

```
1  P1=0.3;//pressure of gas A in atm//
2  VA=50;//volume of gas A in ml//
3  V=500;//Volume of vessel in ml//
4  PA=P1*VA/V;//Pressure of gas A in vessel//
5  printf('Pressure of gas A in vessel=PA=%fatm',PA);
6  P2=0.4;//pressure of gas B in atm//
7  VB=250;//volume of gas B in ml//
8  PB=P2*VB/V;//Pressure of gas A in vessel//
9  printf('\nPressure of gas B in vessel=PB=%fatm',PB);
10 P=PA+PB;//Total pressure in vessel in atm//
11 printf('\nTotal pressure in vessel=P=%fatm',P);
```

Scilab code Exa 4.8 Density of hydrogen

```
1 printf('The volume of 1 mole of H2 at 1 atm and
    273.15K=22.415 Litres');
2 printf('\nThe volume at 0.5atm is obtained by
    considering the constancy of PV');
3 P1=1;
4 V1=22.415;
5 P2=0.5;
```

```
6  V2=(P1*V1)/P2;//Volume at 0.5atm in litres//
7  printf('\nVolume at 0.5atm of H2 at 273.15K=V2=
       %fLitres',V2);
8  MH2=2;//molecular weight of H2//
9  DH2=MH2/V2;//density of H2 in gram per litre//
10 printf('\nDensity of H2=DH2=%fgram per litre',DH2);
```

Scilab code Exa 4.9 Density of hydrogen

```
1  printf('One mole of H2 Occupies 22.415Litres at
       273.15K');
2  printf('\nThe volume at 300K is obtained by
       considering the constancy of V/T');
3  T1=273.15;
4  V1=22.415;
5  T2=300.15;
6  V2=(V1/T1)*T2;//Volume at 300K in litres//
7  printf('\nVolume of 1mole of H2 at 300.15K=V2=
       %fLitres',V2);
8  MH2=2;//molecular weight of H2//
9  DH2=MH2/V2;//density of H2 in gram per litre//
10 printf('\nDensity of H2=DH2=%fgram per litre',DH2);
```

Scilab code Exa 4.10 Relative density

```
1  printf('Density is proportional to molecular weight'
       );
2  printf('\nRelative density of O2 with respect to H2
       is 32/2=16.');
3  t1=12;//time for certain volume of gas to stream
       through hole in mins//
4  p2=16;//Relative density of O2 w.r.t H2//
```

```
5 t2=15;//time for same volume(as gas) of oxygen to
    stream through hole in mins//
6 p1=((t1/t2)^2)*p2;//according to graham's law//
7 printf('\nRealtive density of gas to oxygen=p1=%f',
    p1);//here the answer given in textbook is
    wrongly printed the actual answer is the one we
    got here through execution//
```

Scilab code Exa 4.11 Velocities of Oxygen

```
1 T=320;//47C in kelvin//
2 R=8.31*10^7;//Universal gas constant in erg per
    degree per mole//
3 M=32;//molecular weight of O2 in gram per mole//
4 C2=(3*R*T)/M;//mean square velocity of Oxygen in (cm
    /sec)^2//
5 Crms=sqrt(C2);//Root mean square velocity of Oxygen
    in cm/sec//
6 printf('Root mean square velocity of Oxygen=Crms=
    %fcm/sec',Crms);
7 Cm=sqrt(8*R*T/(%pi*M));//mean velocity of Oxygen in
    cm/sec//
8 printf('\nMean velocity of Oxygen=Cm=%fcm/sec',Cm);
9 Cmpv=sqrt(2*R*T/M);//mean probable velocity in cm/
    sec//
10 printf('\nMean probable velocity of Oxygen=Cmpv=%fcm
    /sec',Cmpv);//in textbook in Cmpv value it is
    misprinted as 10^9 but it is actually 10^4//
```

Scilab code Exa 4.12 Velocities of Gas

```
1 P=10^6;//pressure of gas in dyn per cm^2//
2 p=0.00333;//density of gas in gram per cm^3//
```

```
3 C2=3*P/p;//mean square velocity of gas in (cm/sec)
    ^2//
4 Crms=sqrt(C2);//Root mean square velocity of Oxygen
    in cm/sec//
5 printf('Root mean square velocity of Gas=Crms=%fcm/
    sec',Crms);
6 Cm=Crms/1.085;//mean velocity of Gas in cm/sec//
7 printf('\nMean velocity of Oxygen=Cm=%fcm/sec',Cm);
8 Cmpv=Cm/1.128;//mean probable velocity in cm/sec//
9 printf('\nMean probable velocity of Oxygen=Cmpv=%fcm
    /sec',Cmpv);
```

Scilab code Exa 4.13 mean free path

```
1 printf('Mean free path is inversely proportional to
    N which is proportional to pressure');
2 L1=5.8*10^-6;//mean free path of N2 at NTP in cm//
3 K=58;//preesure is raised 58 times so factor is 58//
4 L2=L1/K;//mean free path of N2 at 58atm pressure in
    cm//
5 printf('\nMean free path of N2 at 58atm pressure
    =1*10^-7cm');
```

Scilab code Exa 4.14 Number of collissions

```
1 T=273;//temperature 0C in kelvin//
2 R=8.31*10^7;//Universal gas constant in erg per
    degree per mole//
3 M=28;//molecular weight of N2 in gram per mole//
4 printf('Since 22.4 Litres of Nitrogen gas at 0C and 1
    atm pressure will contain 6.023*10^23 Molecules.')
    ;
```

```
5 N=2.69*10^19;//no. of molecules in molecules per cm
    ^3//
6 G=3.78*10^-8;//collision diameter in cm//
7 K=sqrt(%pi*R*T/M);
8 Z11=2*N^2*G^2*K;//number of collisions per second of
     Nitrogen at 0C and 1atm//
9 printf('\nNumber of molecular collisions per second
    of Nitrogen at 0C and 1atm=%f=10.43*10^28
    molecular collisions per sec per cm^3',Z11);
```

Scilab code Exa 4.15 Collision diameter

```
1 T=273;//temperature 0C in kelvin//
2 R=8.31*10^7;//Universal gas constant in erg per
    degree per mole//
3 M=28;//molecular weight of N2 in gram per mole//
4 printf('Since 22.4Litres of Nitrogen gas at 0C and 1
    atm pressure will contain 6.023*10^23Molecules.')
    ;
5 N=2.69*10^19;//no. of molecules in molecules per cm
    ^3//
6 Cm=sqrt(8*R*T/(%pi*M));//mean velocity of Nitrogen
    in cm/sec//
7 printf('\nMean velocity of Nitrogen=Cm=%fcm/sec',Cm)
    ;
8 V=22400;//volume of nitrogen in cm^3//
9 p=M/V;//Density of nitrogen in gram per cm^3//
10 printf('\nDensity of Nitrogen=p=%f=1.25*10^-3gram
    per cm^3',p);
11 n=10.99*10^-5;//Viscosity of N2 in poise//
12 L=(3*n)/(Crms*p);//mean free path of nitrogen in cm
    //
13 printf('\nMean free path of Nitrogen=L=5.81*10^-6cm'
    );
14 G=sqrt(1/(1.414*%pi*L*N));//Collision diameter of
```

```
    Nitrogen in cm//
15 printf('\nCollission diameter of Nitrogen=G
    =3.80*10^-8cm');
16 K=sqrt(%pi*R*T/M);
17 Z11=2*N^2*G^2*K;//number of collisions per second of
     Nitrogen at 0C and 1atm//
18 printf('\nNumber of molecular collisions per second
    of Nitrogen at NTP=%f=10.52*10^28molecular
    collisions per sec per cm^3',Z11);
```

Scilab code Exa 4.16 Change in internal energy

```
1 T1=27;//initial temperature in C//
2 T2=177;//final temperature in C//
3 printf('NH3 being a nonlinear molecule has 3
    translational,3 rotational and 6 vibrational
    degrees of freedom.');
4 printf('\nCv=3*0.5*R+3*0.5*R+6*R=9*R');
5 Cv=18;//Molar heat capacity in cal per deg per mol//
6 dU=Cv*(T2-T1);//Change in internal energy of a mole
    in cal per mole//
7 printf('\nChange in internal energy of a mole of NH3
    =dU=%fcal per mole',dU);
8 printf('\nThe actual increase in energy may not be
    2700cal per mol\nbecause at the given temperature
    ,none or only some of the vibrational degrees of
    freedom may be contributing to the total energy.'
    );//answer should come as 2700 not 2400,it was
    just misprinted//
```

Scilab code Exa 4.17 Degree of vibrational freedom

```
printf('CH4 being a nonlinear molecule has 3
    translational,3 rotational and 9 vibrational
    degrees of freedom.');
printf('\nCv=3*0.5*R+3*0.5*R+9*R=12*R');
Cv=24;//Molar heat capacity in cal per degree per
    mol//
printf('\nActual Cv is 16cal per degree per mol');
R=2;
Cvr=16-R;//Real molar heat capapcity in cal per
    degree per mole//
printf('\nReal molar heat capapcity of a mole of CH4
    =Cvr=%fcal per degree per mole',Cvr);
printf('\nThe Real molar heat capacity at constant
    volume is 10cal less than the theoretical value.\
    nSince each vibrational degree of freedom can
    contribute 2cal,this means that 5 vibrational
    degrees\nare not contributing at the given
    temperature.');
```

Scilab code Exa 4.18 Lowest temperature

```
a=3.60;//Van der Waals constant for CO2 in L^2 atm
    per mol^2//
b=4.30*10^-2;//Van der Waals constant for CO2 in
    litre per mol//
N=300;//No. of moles of CO2 the cylinder contains//
V=100;//volume of cylinder in litres//
P=150;//Maximum pressure the cylinder can withstand
    in atm//
R=0.082;
K1=P+(N^2*a/V^2);
K2=V-(N*b);
T=(K1*K2)/(N*R);//The lowest temperature at which
    cylinder can explode in Kelvin//
printf('The lowest temperature at which cylinder can
```

```
explode=T=%fK',T);
```

Scilab code Exa 4.19 Viscosity of liquids

```
tA=280;//time of flow for liquid A in seconds//
tB=200;//time of flow for liquid B in seconds//
pA=1;//density of liquid A in gram per cm^3//
pB=1.1;//density of liquid B in gram per cm^3//
h=10;//height of liquid responsible for the flow in
   cm//
g=980;//gravity constant in dyns//
V=1;//volume of liquid in ml//
L=10;//length of the capillary in cm//
r=0.1;//radius of the capillary in cm//
PA=h*pA*g;//Pressure of liquid A//
PB=h*pB*g;//Pressure of liquid B//
nA=(%pi*PA*tA*r^4)/(8*L*V);//Viscosity of Liquid A
   in centipoise//
printf('\nViscosity of Liquid A=nA=%fcentipoise',nA)
   ;
nB=(%pi*PB*tB*r^4)/(8*L*V);//Viscosity of Liquid B
   in centipoise//
printf('\nViscosity of Liquid B=nB=%fcentipoise',nB)
   ;
```

Scilab code Exa 4.20 Depression in capillary

```
ST=520;//surface tension of mercury in dyn per cm//
d=13.6;//density of mercury in gram per cm^3//
g=980;//gravity constant in dyns//
r=0.1;//radius of the capillary tube in cm//
h=(ST*2)/(g*r*d);//Depression observed in capillary
   tube in cm//
```

```
6 printf('Depression observed in capillary tube=h=%fcm
    ',h);//the answer is given wrong in textbook,it
    should actually be double the one given//
```

Scilab code Exa 4.21 Surface excess concentration

```
1 T=293;//temperature 20C in kelvin//
2 R=8.31*10^7;//Universal gas constant in erg per
    degree per mole//
3 dr=165;//Change of surface tension in erg per cm^2
    per mol litre//
4 C=0.06;//concentration we are considering in M//
5 t=(C*dr)/(R*T);//surface excess concentration of
    phenol in mol per cm^2//
6 printf('surface excess concentration of phenol=t
    =4.08*10^-10mol per cm^2');
```

Scilab code Exa 4.22 length of a molecule

```
1 M=256;//Molecular weight of acid in grams//
2 w=2.56*10^-5;//weight of palmitic acid in grams//
3 N=w/M;//No. of molecules of acid//
4 A=123;//Total area occupied in cm^2//
5 AM=A/N;//Area per molecule in cm^2//
6 printf('Area per molecule=20.4*10^-16cm^2.\nThis is
    the area of crosssection A for a vertical
    position.');
7 V=w/0.81;//Volume of acid in cm^3//
8 VM=V/N;//Volume of one molecule of acid in cm^3//
9 L=VM/AM;//Length of molecule in cm//
10 printf('\nLength of a molecule=25.7*10^-8cm');
```

Scilab code Exa 4.23 Molecular weight

```
1 T=298;//Temperature in kelvin//
2 ST=0.2;//Lowered surface tension in dyn per cm//
3 K=1.37*10^-16;//Boltzman's constant//
4 AM=(K*T)/ST;//Area per molecule on the surface in cm
    ^2//
5 A=300;//Total area occupied in cm^2//
6 N=A/AM;//no. of molecules//
7 W=3*10^-7;//weight of insoluble substance in grams//
8 w=W/N;//weight of one molecule in grams//
9 N1=6.023*10^23;
10 MW=w*N1;//Molecular weight of substance in grams//
11 printf('Molecular weight of substance=MW=%f=123',MW)
    ;
```

Scilab code Exa 4.24 Surface area

```
1 MW=461;//molecular weight of lead iodide in  grams//
2 CR1=3000;//initial count rate in count per minute//
3 CR2=900;//final count rate in count per minute//
4 CR=CR1-CR2;
5 printf('The count for lead iodide as absorbed=CR=
    %fcount per minute',CR);
6 printf('\nThe ratio of weights of lead iodide and
    radio lead iodide in solution is equal to that of
     the same ratio on surface');
7 printf('\nWeight of lead iodide in solution=0.0014
    grams');
8 printf('\nWeight of radio lead iodide is
    proportional to the count.\nWeight of lead iodide
     on the surface=0.0014*21/9.\nMolecular weight of
```

```
 lead iodide=461.\nArea of the surface per gram
=4266cm^2 g^-1');
```

Scilab code Exa 4.25 Area per gram

```
1 printf('From the linear plot of the langmuir
    isotherm the intercept Xm=1/0.19=5.26 milligrams')
    ;
2 Xm=5.26*10^-3;
3 printf('\nThis is the weight of N2 that forms a
    unimolecular layer of 2g charcoal.');
4 MW=28;//molecular weight of N2//
5 N=Xm*6.023*10^23/MW;//No. of molecules of N2//
6 TA=N*16*10^-16;//Total area in cm^2//
7 A=TA/2;//Area per gram in cm^2//
8 printf('\nArea of N2 per gram=%fcm^2',A);
```

Scilab code Exa 4.26 Area per gram

```
1 printf('From the linear plot of the langmuir
    isotherm the intercept=0.35*10^-3 and slope
    =9.47*10^-2');
2 printf('\nVolume is the inverse of summation of
    intercept and slope and that is 10.52cc');
3 Vm=10.52;//volume in cc//
4 m=Vm/22400;//No. of moles of N2//
5 N=m*6.023*10^23;//No. of molecules of N2//
6 TA=N*16*10^-16;//Total area in cm^2//
7 A=TA/17.5;//Area per gram in cm^2//
8 printf('\nArea of N2 per gram=%fcm^2',A);
```

Scilab code Exa 4.28 Surface area

```
d=13.56;//density of mercury in gr per cm^3//
V=1/d;//Volume of mercury in cm^3//
D=0.07*10^-4;//Diameter of the globule in cm//
r=D/2;//radius of globule in cm//
printf('One globule of mercury occpies a volume of
    1.33*3.14*r^3cm^3\nSurface area of one globule
    =4*3.14*r^2');
Vg=1.33*3.14*r^3;//volume of one globule in cm^3//
y=0.0738/Vg;//No of globules in 0.0738 volume//
printf('\nNo. of globules in 0.0738cm^3=y=%f',y);
SA=y*4*3.14*r^2;//Surface area of y globules in cm
    ^2//
printf('\nSurface area of y globules=SA=%fcm^2',SA);
```

Scilab code Exa 4.29 Avagadro Number

```
T=300;//temperature in kelvin//
R=8.31*10^7;//Universal gas constant in ergs//
r=2*10^-5;//average radius of particles in cm//
h=4.15*10^-3;//Vertical seperation in cm//
p=1.21;//density of latex in gram per cm^3//
g=980;//gravity constant in dynes//
printf('Since the dispersion medium is water its
    density is p1=1.\nwhen the system equilibrated
    average number of colloidal particles seen in the
     field is halved so N0/N=2.\nthe required
    expression is derived based on kinetic energy of
    particles');
p1=1;//density of water//
L=log(2)*0.75*(R*T)/(%pi*g*h*(p-p1)*r^3);
printf('\nValue of Avagadro number is L=%f
    =6.037*10^23molecules per mol.',L);
```

Scilab code Exa 4.30 Diameter of particle

```
Vf=117.857*10^-9;//Volume falling within field of
   view in ml//
AN=9.66;//Average no. of particles per count//
N=AN/Vf;//No. of particles per count//
printf('No .of particles per ml=N=%f',N);
W=1.5*10^-7;//Weight of iron oxide per ml//
w=W/N;//weight of one particle in grams//
printf('\nWeight of one particle=w=1.83*10^-15grams'
   );
d=5.2;//density of iron oxide in g per cm^3//
V=w/d;//Volume of one particle in cm^3//
printf('\nVolume of one particle=V=3.52*10^-16cm^3')
   ;
R=2.032*10^-5;//radius of particle in cm//
printf('Radius of particle=R=2.032*10^-5cm\nDiameter
    of particle=4.064*10^-5cm');
```

Scilab code Exa 4.31 Electrokinetic potential

```
D=78;//dielectric constant//
V=0.009;//viscosity of suspension in dyn sec per cm
   ^2//
P=3.2;//potential gradient in volt per cm//
t=38.2;
d=0.033;//standard distance between electrodes in cm
   //
u=90000;
EP=(4*%pi*V*u*d)/(D*t*P);//Electrokinetic potential
   of the catalyst in volts//
```

```
8 printf('Electrokinetic potential of the catalyst=EP=
    %fvolts',EP);
```

Scilab code Exa 4.32 Zeta potential

```
1 D=80.36;//dielectric constant//
2 V=0.01;//viscosity of suspension in dyn sec per cm
    ^2//
3 P=10;//potential gradient in volt per cm//
4 v=3*10^-3;//observed velocity in cm per sec//
5 u=90000;
6 EP=(4*%pi*V*u*v)/(D*P);//Zeta potential of the
    catalyst in volts//
7 printf('Zeta potential of the catalyst=EP=%fvolts',
    EP);
8 printf('\nThe effective thickness of the double
    layer can be taken to be 1cm');
9 e=9*10^-4;
10 r=0.5*10^-4;
11 N=4*%pi*e*r^2;//total no. of charges carried by a
    particle//
12 printf('\nTotal no. of charges carried by a particle
    =N=2.83*10^-11');
```

Scilab code Exa 4.33 Flow of water

```
1 D=80.36;//dielectric constant//
2 V=0.01;//viscosity of suspension in dyn sec per cm
    ^2//
3 P=100;//potential gradient in volt per cm//
4 u=90000;
5 EP=0.03;//Electrokinetic potential of the catalyst
    in volts//
```

```
6 FW=(P*EP*D*3600)/(4*%pi*V*u);//amount of flow of
    water in cm per hour//
7 printf('Amount of flow of water through diaphragm=FW
    =%fcm per hour',FW);
```

Scilab code Exa 4.34 Flow of water

```
1 D=80.36;//dielectric constant//
2 V=0.01;//viscosity of suspension in dyn sec per cm
    ^2//
3 P=40;//potential gradient in volt per cm//
4 r=0.05;//radius of capillary in cm//
5 u=90000;
6 ZP=0.05;//Zeta potential of the catalyst in volts//
7 FW=(P*ZP*D*3600*r^2)/(4*V*u);//amount of flow of
    water in cc per hour//
8 printf('Amount of flow of water through diaphragm=FW
    =%fcc per hour',FW);
```

Scilab code Exa 4.35 Concentrations and EMF

```
1 C1=5*10^-4;
2 C2=2.5*10^-4;
3 x=(C1^2)/(C2+(2*C1));//The amount of Na+ transported
    at equilibrium in M//
4 printf('The amount of Na+ transported at equilibrium
    =x=2*10^-4M');
5 NaR=C2+x;//Na+ on RHS//
6 printf('\nNa+ on RHS=4.5*10^-4M.\nCl- on RHS=x
    =2*10^-4M.\nNa+ on LHS=Cl- on LHS=C1-x=3*10^-4M')
    ;
7 printf('\nE is in volts and F in coulombs.for
    homogeneity of units either R should be expressed
```

```
    in coulombs or F in calories.F is 96500C or
    23060cal.');
F=23060;
n=1;
T=300;//temperature in kelvin//
R=2;
K=1.5;
E=(R*T*log(K))/(n*F);//Emf across membrane in volts
    //
printf('\nEmf across membrane=E=%fvolts',E);
```

Scilab code Exa 4.36 Concentrations

```
C1=0.04;
C2=0.02;
x=(C1^2)/(C2+(2*C1));//The amount of Na+ transported
    at equilibrium in M//
printf('The amount of Na+ transported at equilibrium
    =x=%fM',x);
NaR=C2+x;//Na+ on RHS//
printf('\nNa+ on RHS=NaR=%fM',NaR);
NaL=C1-x;//Na+ on LHS//
printf('\nNa+ on LHS=NaL=%fM',NaL);
```

Scilab code Exa 4.37 unit cell length and wavelength

```
MW=58.45;//Molar weight of NaCl in grams//
d=2.17;//density of NaCl in g/cc//
MV=MW/d;//Molar volume in cc//
printf('Molar Volume of NaCl=MV=%fcc',MV);
printf('\nThis must contain 6.023*10^23 NaCl units.\
    nIn one unit cell of NaCl there are 8 corner Na+
    ions and 6 on the face centres.\nThe number of Na
```

```
    + ions in one unit cell is 8*1/8+6*1/2=4.\nThere
    are 12Cl- ions on the edges,and one in the centre
    .\nThe number of Cl- ions are 12*1/4+1=4 ');
6 printf('\nThe volume of the unit cell containing 4
    NaCl units=179*10^-24cc');
7 a=5.63*10^-8;//unit cell length in cm//
8 printf('\nUnit cell length of NaCl crystal=a
    =5.63*10^-8cm');
9 Id=a/2;//Interionic distance in cm//
10 printf('\nInterionic distance in the crystal=Id
    =2.815*10^-8cm');
11 Q=5.9;//glancing angle in degrees//
12 L=2*Id*sin(Q*%pi/180)*10^8;//wavelenth in angstrums
    //
13 printf('\nWavelength of the Xrays used=L=%fAngstrums
    ',L);
```

Scilab code Exa 4.39 type of cubic unit cell

```
1 N=2;//No. of atoms or unit cells in BCC structure//
2 L=6.023*10^23;//Avagadro number//
3 a=4.291*10^-8;//Unit cell edge length in cm//
4 Na=23;//weight of Na//
5 p=(N*Na)/(L*a^3);//density of Na at room temperature
    in g/cm^3//
6 printf('Density of Na at room temperature=p=%fg/cm^3
    ',p);
7 P=p*1.0398;//density of Na at -195degrees
    temperature in g/cm^3//
8 printf('\nDensity of Na at -195degrees temperature=P
    =%fg/cm^3',P);
9 a1=5.35*10^-8;//unit cell edge length in cm//
10 N1=(P*L*a1^3)/(Na);//No. of unitcells at -195degrees
    //
11 printf('\nNumber of unitcells at -195degrees=N1=%f',
```

```
    N1);
12 printf('\nAt -195degrees temperature Na have 4
    unitcells which means it assumes an FCC structure
    .');
```

Chapter 5

THERMODYNAMICS

Scilab code Exa 5.1 Maximum work

```
1 P1=10;//initial pressure in atm//
2 P2=1;//final pressure in atm//
3 Wrev=0.0821*273*log(P1/P2);//maximum work required
    for the expansion of gas in litre-atm//
4 printf('Maximum work required for the expansion of 1
    mol of ideal gas from 10atm to 1atm=Wrev=%flitre
    atm',Wrev);
5 printf('\nIf the gas is now compressed back from 1
    atm to 10atm under isothermal conditions,Wrev
    =-51.608530litre atm');
```

Scilab code Exa 5.2 Maximum work

```
1 n=5;//no. of moles of Benzene//
2 R=8.314*10^7;//Universal gas constant//
3 K=80;//Evaporated temperature of benzene in
    centigrades//
4 T=270+K;//evaporated temperature of benzene in
    kelvins//
```

```
5 Wrev=n*R*T;//Maximum work done in ergs//
6 printf('Maximum work done=Wrev=%fergs=1.454*10^11
    ergs',Wrev);
```

Scilab code Exa 5.3 Enthalpy change

```
1 w=0.454;//weight of TNT in grams//
2 T=298;//temperature in kelvin//
3 R=2*10^-3;
4 dn=5;
5 m=w/227;//mol of TNT exploded//
6 printf('mol of TNT exploded=%fmol',m);
7 H=1.64;//Heat liberated in kcal//
8 dU=-H/m;
9 printf('\ndU=%fKcal per mol',dU);
10 dH=dU+(R*T*dn);
11 printf('\ndH=%fKcal per mol',dH);
```

Scilab code Exa 5.4 Final pressure of the system

```
1 dH=-817;
2 dU=-820;
3 P1=1;//initial pressure in atm//
4 V=1;//volume in litre//
5 K=(1.99*10^-3)/0.082;//multiplying factor to convert
    litre atm to calories//
6 P2=P1+((dH-dU)/(V*K));//final pressure in atm//
7 printf('Final pressure of the system=P2=%fatm',P2);
8 printf('\nIn this problem P1 and P2 are in atm and V
    being in litres,The VdP term in litre atm.\ndH
   and dU are in Kcal and so the VdP term is
   converted into Kcal.\nIt is seen that the
   pressure developed is enormous.\nThis takes place
```

```
 in a confined space,an explosion occurs.\nThe
final pressure P2 can also be calculated from the
 ideal gas equation PV=nRT which gives the same
result.');//in textbook the answer given is bit
wrong and it should be one we get through
execution//
```

Scilab code Exa 5.5 Enthalpy change

```
1 dHfFe2O3=-196.5;//dHf value of Fe2O3 in kcal per mol
   //
2 dHfCO2=-94.05;//dHf value of CO2 in kcal per mol//
3 dHfCO=-26.41;//dHf value of CO in kcal per mol//
4 dH298=(3*dHfCO2-dHfFe2O3-3*dHfCO);//enthalphy change
    at 298K in Kcal//
5 printf('Enthalpy change for the reduction of Fe2O3
   by Co at 298K=%fKcal',dH298);
```

Scilab code Exa 5.6 Standard Enthalpy of formation

```
1 dHfH2O=-68.32;//dHf value of H2O in kcal per mol//
2 dHfCO2=-94.05;//dHf value of CO2 in kcal per mol//
3 dH298=-208.34;//enthalphy change at 298K in Kcal//
4 dHfCH3COOH=(2*dHfH2O+2*dHfCO2-dH298);//dHf value of
   CH3COOH in Kcal per mol//
5 printf('Standard enthalpy of formation of CH3COOH=
   %fKcal per mol',dHfCH3COOH);
```

Scilab code Exa 5.7 Enthalpy change

```
T=298;//temperature in kelvin//
R=1.987*10^-3;
dn=-4;
dU=-1148.93;//Internal energy change of n-Heptane in
    kcal per mol//
dHf=dU+(R*T*dn);//dHf value of C7H16 in Kcal per mol
   //
printf('dHf value of C7H16=dHf=%fKcal per mol',dHf);
dHfH2O=-68.32;//dHf value of Fe2O3 in kcal per mol//
dHfCO2=-94.05;//dHf value of CO2 in kcal per mol//
dHfC7H16=(8*dHfH2O+7*dHfCO2-dHf);//dHf value of
   CH3COOH in Kcal per mol//
printf('\nStandard enthalpy of formation of C7H16=
   %fKcal per mol',dHfC7H16);
```

Scilab code Exa 5.8 Heat of formation

```
dHf=-67.63;//enthalpy change value in kcal//
dHfCO2=-94.05;//Heat of formation value of CO2 in
   kcal//
dHfCO=dHfCO2-dHf;//Heat of formation value of CO in
   Kcal//
printf('Heat of formation of CO=%fKcal',dHfCO);
```

Scilab code Exa 5.9 Enthalpy change

```
dHfDiam=-94.50;//heat of formation value of Diamond
   in kcal//
dHfGrap=-94.05;//Heat of formation value of Graphite
    in kcal//
dHf=dHfGrap-dHfDiam;//Enthalpy change when graphite
   converted to diamond in Kcal//
```

```
4 printf('Enthalpy change when graphite converted to
    diamond=%fKcal',dHf);
```

Scilab code Exa 5.10 Standard Enthalpy of formation

```
1 dHfH2O=-68.32;//dHf value of H2O in kcal per mol//
2 dHfCO2=-94.05;//dHf value of CO2 in kcal per mol//
3 dH298=-208.34;//enthalphy change at 298K in Kcal//
4 dHfCH3COOH=(2*dHfH2O+2*dHfCO2-dH298);//dHf value of
    CH3COOH in Kcal per mol//
5 printf('Standard enthalpy of formation of CH3COOH=
    %fKcal per mol',dHfCH3COOH);
```

Scilab code Exa 5.11 Standard Enthalpy of formation

```
1 dHfZnSO4l=-36.43;//Standard heat of formation of
    ZnSO4 in kcal//
2 dHfH2SO4l=-193.91;//Standard heat of formation of
    H2SO4 in kcal//
3 dHfZnSO4aq=-19.45;//Heats of Dilution of ZnSO4 in
    kcal//
4 dHfH2SO4aq=-22.99;//Heats of Dilution of H2SO4 in
    kcal//
5 dH=dHfZnSO4l+dHfH2SO4l+dHfH2SO4aq;
6 dHf298=dH-dHfZnSO4aq;//Standarad enthalphy of
    formation of ZnSO4 at 298K in Kcal//
7 printf('Standard enthalpy of formation of ZnSO4 at
    298K=%fKcal',dHf298);
```

Scilab code Exa 5.12 Heat of formation of water vapour

```
CvH2=6.95*10^-3;//Mean molar capacity of H2 in Kcal
    per deg//
CvO2=6.97*10^-3;//Mean molar capacity of O2 in Kcal
    per deg//
CvH2O=8.7*10^-3;//Mean molar capacity of H2O in Kcal
     per deg//
dCv=CvH2O-CvH2-0.5*CvO2;//Net mean molar capapcity
    in Kcal per deg//
printf('Net mean molar capacity=dCv=%fKcal per deg',
    dCv);
dHf=-57.8;//Standard heat of formation of water
    vapour in Kcal//
dHf373=dHf+(dCv*(373-298));//Heat of formation of
    water vapour at 373K in Kcal//
printf('\nHeat of formation of water vapour at 373K=
    %fKcal',dHf373);//here the answer is written
    wrong in textbook the correct answer is given
    here//
```

Scilab code Exa 5.13 Enthalpy formation of CO2

```
CvCO2=1.331;//Mean molar capacity of CO2 in Kcal per
     deg//
CvC=6.714*10^-3;//Mean molar capacity of C in Kcal
    per deg//
CvO2=-77.09*10^-7;//Mean molar capacity of O2 in
    Kcal per deg//
T1=300;//Initial Temperature in kelvin//
T2=400;//final temperature in Kelvin//
dHf400=-94.06;//Enthalpy change in the formation of
    CO2 at 400k in Kcal//
dHf300=dHf400-((CvCO2*(T2-T1))-(0.5*CvC*(T2^2-T1^2))
    -(0.33*CvO2*(37*10^6)))*10^-3;//Enthropy of
    formation of CO2 at 300K in Kcal//
printf('\nEnthropy of formation of CO2 at 300K=
```

```
%fKcal',dHf300);//in textbook the answer is not
    having negative answer//
```

Scilab code Exa 5.14 Enthalpy change

```
1 dHfNH3=-11.04;//Standard heat of formation of NH3 in
      kcal//
2 dHfH2O=-57.80;//Standard heat of formation of H2O in
      kcal//
3 dHfNO=21.60;//Standard heat of formation of NO in
    kcal//
4 dHfO2=0;//Standard heat of formation of O2 in Kcal//
5 dH=4*dHfNO+6*dHfH2O-4*dHfNH3-5*dHfO2;//Enthalpy
    change for the oxidation of NH3//
6 printf('Enthalpy change for the oxidation of NH3 at
    298K=%fKcal',dH);
```

Scilab code Exa 5.15 Enthalpy change

```
1 T=773;//temperature in kelvin//
2 dH298=-216240;//Enthalpy change for the oxidation of
      NH3 in cal//
3 CvO2=6.148+T*3.102*10^-3-(T^2)*9.23*10^-7;//heat
    capacity of O2 in cal deg^-1 mol^-1//
4 CvH2O=7.219+T*2.374*10^-3+(T^2)*2.67*10^-7;//Heat
    capacity of H2O in cal deg^-1 mol^-1//
5 CvNO=6.50+T*1*10^-3;//Heat capacity of NO in cal per
      deg per mol//
6 CvNH3=6.189+T*7.887*10^-3-(T^2)*7.28*10^-7;//Heat
    capacity of H2O in cal deg^-1 mol^-1//
7 dCv=4*CvNO+6*CvH2O-4*CvNH3-5*CvO2;//Heat capacity
    change for oxidation//
8 da=13.818;
```

```
db=-28.814*10^-3;
dc=91.29*10^-7;
T1=298;//temperature in kelvin//
dH773=dH298+(T-T1)*da+(T^2-T1^2)*0.5*db+(T^3-T1^3)
   *0.33*dc;//Enthalpy change for the oxidation of
   NH3 at 773k in cal//
printf('\nEnthalpy change for the oxidation of NH3
   at 773K=%fcal=-215.69Kcal',dH773);//here the
   answer is slightly different//
```

Scilab code Exa 5.16 Enthalpy change

```
ECH=99;//bond energy of CH bond in Kcal//
EClCl=58;//bond energy of ClCl bond in Kcal//
ECCl=78;//bond energy of CCl bond in Kcal//
EHCl=103;//bond energy of HCl bond in Kcal//
dE=4*ECH+4*EClCl-4*ECCl-4*EHCl;//Net change in bond
   energy in kcal//
printf('Enthalpy change of the reaction=dE=%fKcal',
   dE);
```

Scilab code Exa 5.17 Maximum temperature

```
T1=298;//initial temperature in kelvin//
pO2=0.2;//percentage of oxygen in air//
pN2=0.8;//percentage of nitrogen in air//
dH298=-310;//Heat of combustion of acetylene in Kcal
   //
printf('The combustion of acetelyne proceeds
   according to the equation C2H2+2.5 O2 = 2CO2+H2O
   ,\nHeat of combustion of acetylene=dH298=-310KCal
   .');
```

```
6 printf('\nThe scheme of calculation can be
    represented as Reactants at 298 = Products at T2K
    .\nThe gases present in the flame zone after
    combustion are CO2,H2O and unreacted N2 of the
    air.');
7 printf('\nSince 2.5mol of O2 have been utilized for
    combustion,4*2.5mol i.e 10mol of N2 are present
    in the flame zone.\nThe heat generated at 298K,
    dH298 is utilized in raising the products at 298K
     to a temeprature of T2K.');
8 printf('\nThe Heat capacity equations given in the
    question can be solved and after solving we will
    get a quadratic equation that is T2^2+4511*T2
    -2.273*10^7=0 \nMaximum temperature reached by an
     oxy-acetylene flame at constant pressure=T2
    =3015.0000K.');
```

Scilab code Exa 5.18 Maximum temperature and pressure

```
1 dH=-57800;//Enthalpy change in cal//
2 R=1.99;//universal gas constant//
3 T=298;//temperture in kelvin//
4 dn=-0.5;//change in no. of moles//
5 dU=dH-(R*T*dn);//heat of combustion in cal//
6 printf('The air used contains 2 mol of N2.\ndU
    =-57500cal.');
7 CpN2=8.3;//Cp value of N2//
8 CpH2O=11.3;//Cp value of H2O//
9 CvN2=CpN2-R;//Cv value of N2//
10 CvH2O=CpH2O-R;//Cv value of H2O//
11 printf('\nCv value of N2=CvN2=%fKcal deg^-1 mol^-1',
    CvN2);
12 printf('\nCv value of H2O=CvH2O=%fKcal deg^-1 mol^-1
    ',CvH2O);
13 printf('\nSolving integration we get T2=2940K.The
```

```
    maximum pressure can be calculated from PV=nRT
    equation.');
P1=1;//initial pressure in atm//
n1=3.5;
n2=3;
T2=2940;//final temperature in Kelvin//
P2=(P1*n2*T2)/(n1*T);//maximum pressure in atm//
printf('\nMaximum pressure of the reaction=P2=%fatm'
    ,P2);
```

Scilab code Exa 5.20 Maximum possible efficiency

```
printf('The maximum possible efficiency is obtained
    only in a reversible carnots cycle according to
    which ME=dT/T.');
T=300;//initial temperature of steam engine in
    kelvin//
T1=373;//operating temperature in kelvin//
ME1=(T1-T)/T1;//maximum possible efficiency for
    temperature range of 300k to 373k//
printf('\nMaximum possible efficiency for operating
    temperature between 300K and 373K=ME1=%f',ME1);
T2=630;//operating temperature in kelvin//
ME2=(T2-T)/T2;//maximum possible efficiency for
    temperature range of 300k to 630k//
printf('\nMaximum possible efficiency for operating
    temperature between 300K and 630K=ME1=%f',ME2);
T3=510;//operating temperature in kelvin//
ME3=(T3-T)/T3;//maximum possible efficiency for
    temperature range of 300k to 510k//
printf('\nMaximum possible efficiency for operating
    temperature between 300K and 510K=ME3=%f',ME3);
```

Scilab code Exa 5.22 entropy change

```
T1=300;//initial temperature in kelvin//
T2=400;//final temperature in kelvin//
P1=2;//initial pressure in atm//
P2=10;//final pressure in atm//
R=1.99;
n=5;//no.of moles//
Cv=6.95;
dS=n*Cv*2.303*log10(T2/T1)-n*2.303*R*log10(P2/P1);
printf('Change in entropy=dS=%feu',dS);
```

Scilab code Exa 5.23 Entropy change

```
Lv=6896;//Latent heat of vapourization in cal per
   mol//
Tb=341.7;//Boiling temperature in kelvin//
dS=Lv/Tb;//entropy change accompanying the
   vapourization in eu//
printf('Entropy change accompanying the
   vapourization=dS=%feu or cal per deg',dS);
```

Scilab code Exa 5.24 Entropy change

```
T1=300;//initial temperature in kelvin//
T2=600;//final temperature in kelvin//
T3=373;//initial temperature in kelvin//
T4=746;//final temperature in kelvin//
Cv=6.09;//molar heat capacity in cal per deg//
dS2=Cv*2.303*log10(T2/T1);//change in entropy for
   temperature change between 300k to 600k//
printf('Change in entropy for temperature change
   between 300k to 600k=dS2=%fcal per deg',dS2);
```

```
8 dS4=Cv*2.303*log10(T4/T3);//change in entropy for
    temperature change between 373k to 746k//
9 printf('\nChange in entropy for temperature change
    between 373k to 746k=dS4=%fcal per deg',dS4);
```

Scilab code Exa 5.25 Total Entropy change

```
1 T=300;//initial temperature in kelvin//
2 T1=692;//temperature in kelvin//
3 T2=1180;//temperature in kelvin//
4 T3=1500;//final temperature in kelvin//
5 Lf=1800;//Latent heat of fusion in cal per mol//
6 Tf=692;//temperature of fusion in kelvin//
7 Lv=27700;//Latent heat of vapourization in cal per
    mol//
8 Tv=1180;//temperature of vapourization in kelvin//
9 SH=0.092;//specific heat of Zn in cal per deg per
    gram//
10 w=65.38;//atomic weight of Zn//
11 Cv=w*SH;//molar heat capacity in cal per deg//
12 dS1=Cv*2.303*log10(T1/T);//change in entropy for
    temperature change between 300k to 692k//
13 printf('Change in entropy for temperature change
    between 300k to 692k=dS1=%feu',dS1);
14 dS2=Lf/Tf;//change in entropy in the process of
    fusion in eu//
15 printf('\nChange in entropy in the process of fusion
    =dS2=%feu',dS2);
16 dS3=Cv*2.303*log10(T2/T1);//change in entropy for
    temperature change between 692k to 1180k//
17 printf('\nChange in entropy for temperature change
    between 692k to 1180k=dS3=%feu',dS3);
18 dS4=Lv/Tv;//change in entropy in the process of
    vapourization in eu//
19 printf('\nChange in entropy in the process of
```

```
    vapourization=dS4=%feu',dS4);
20 dS5=Cv*2.303*log10(T3/T2);//change in entropy for
    temperature change between 1180k to 1500k//
21 printf('\nChange in entropy for temperature change
    between 1180k to 1500k=dS5=%feu',dS5);
22 dStotal=dS1+dS2+dS3+dS4+dS5;//total entropy change
    accompanying the process in eu//
23 printf('\nTotal entropy change accompanying the
    process=dStotal=%feu',dStotal);
```

Scilab code Exa 5.26 Entropy change

```
1 printf('This is a spontaneous process.Since dS is
    independent of the manner in which the processes
    are conducted,\nthe above irreversible process
    can be considered to take place reversibly.')
2 T1=300;//initial temperature in kelvin//
3 T2=370;//final temperature in kelvin//
4 Cv=18;//molar heat capacity in cal per deg//
5 dSH2O=-Cv*2.303*log10(T2/T1);//change in entropy of
    H2O for temperature change between 300k to 370k//
6 printf('\nChange in entropy of H2O for temperature
    change between 300k to 370k=dSH2O=%feu',dSH2O);
7 dT=T2-T1;//change in temperature in kelvin//
8 dSthermostat=Cv*dT/T1;//change in entropy of
    thermostat in eu//
9 printf('\nChange in entropy of thermostat=
    dSthermostat=%feu',dSthermostat);
10 dS=dSH2O+dSthermostat;//net entropy chane in eu//
11 printf('\nNet entropy change=dS=%feu',dS);
```

Scilab code Exa 5.27 Standard free energy change

```
dGC2H6O=-41.77;//Standard free energy change of
   C2H6O in Kcal per mol//
dGCO2=-94.26;//Standard free energy change of CO2 in
    Kcal per mol//
dGH2O=-56.69;//Standard free energy change of C2H6O
   in Kcal per mol//
dGO2=0;//Standard free energy change of O2 in Kcal
   per mol//
dG=2*dGCO2+3*dGH2O-dGC2H6O-3*dGO2;//Standard free
   energy change in Kcal//
printf('Standard free energy change accompanying the
    combustion of ethanol at 298K=%fKcal',dG);
```

Scilab code Exa 5.28 Standard free energy change

```
dGCH3COOH=-93.8;//Standard free energy change of
   CH3COOH in Kcal per mol//
dGCH3CH2OH=-41.77;//Standard free energy change of
   CH3CH2OH in Kcal per mol//
dGH2O=-56.69;//Standard free energy change of C2H6O
   in Kcal per mol//
dGO2=0;//Standard free energy change of O2 in Kcal
   per mol//
dG=dGCH3COOH+dGH2O-dGCH3CH2OH-dGO2;//Standard free
   energy change in Kcal//
printf('Standard free energy change accompanying the
    Oxidation of ethanol to acetic acid=%fKcal',dG);
printf('\nSince dG is negative the reaction is
   feasible under these conditions.');
```

Scilab code Exa 5.29 Standard free energy change

```
dGAgCl=-26.22;//Standard free energy change of AgCl
    in Kcal per mol//
dGAgI=-15.85;//Standard free energy change of AgI in
    Kcal per mol//
dGKCl=-97.59;//Standard free energy change of KCl in
    Kcal per mol//
dGKI=-77.03;//Standard free energy change of KI in
    Kcal per mol//
dG=dGAgCl+dGKI-dGAgI-dGKCl;//Standard free energy
    change in Kcal//
printf('Standard free energy change accompanying the
    given reaction=%fKcal',dG);
printf('\nSince dG is positive the reaction is not
    feasible under these conditions but the reverse
    reation is possible.');
```

Scilab code Exa 5.30 Standard Entropy change

```
SFe2O3=21.5;//Standard Entropy of Fe2O3 in cal per
    deg per mol//
SCO=47.3;//Standard Entropy of CO in cal per deg per
    mol//
SFe=6.5;//Standard Entropy of Fe in cal per deg per
    mol//
SCO2=51.1;//Standard Entropy of CO2 in cal per deg
    per mol//
dS=2*SFe+3*SCO2-SFe2O3-3*SCO;//Standard entropy
    change in cal per deg per mol//
printf('Standard entropy change accompanying the
    reduction of Fe2O3 by CO=%fcal per deg per mol',
    dS);
printf('\nHere it will be noticed that dS is very
    small but definitely positive.');
printf('\nThe small value due to the fact that there
    is no change in number of moles of gases\nwhich
```

```
are major contributors to the entropy change.');
```

Scilab code Exa 5.31 Standard Entropy change

```
1 SCaCO3=22.2;//Standard Entropy of CaCO3 in cal per
    deg per mol//
2 SCaO=9.5;//Standard Entropy of CaO in cal per deg
    per mol//
3 SCO2=51.1;//Standard Entropy of CO2 in cal per deg
    per mol//
4 dS=SCaO+SCO2-SCaCO3;//Standard entropy change in cal
     per deg per mol//
5 printf('Standard entropy change in the given
    reaction=%fcal per deg per mol',dS);
```

Scilab code Exa 5.32 Standard Entropy change

```
1 SFe2O3=21.5;//Standard Entropy of Fe2O3 in cal per
    deg per mol//
2 SH2=31.21;//Standard Entropy of H2 in cal per deg
    per mol//
3 SFe=6.5;//Standard Entropy of Fe in cal per deg per
    mol//
4 SH2O=16.75;//Standard Entropy of H2O in cal per deg
    per mol//
5 dS=2*SFe+3*SH2O-SFe2O3-3*SH2;//Standard entropy
    change in cal per deg per mol//
6 printf('Standard entropy change in the given
    reaction=%fcal per deg per mol',dS);
```

Scilab code Exa 5.33 Fugacity

```
T=273;//temperature in kelvin//
P1=1;//pressure in atm//
M=28;//molecular weight of N2 in grams//
printf('For an ideal gas density=M*P/R*T.\nWhere M
   is molecular weight=28.\nTemperature being
   constant,if p1 and p2 are the densities at 1atm
   and 50atm respectively');
P2=1.25;//pressure in atm//
p1=50;//density at 1atm pressure//
p2=p1*P2;
printf('\nIf N2 gas behaved ideally at 273k,the
   ideal pressure Pideal is given by p2*R*T/M');
Pideal=p2*0.0821*T/M;
printf('\nIdeal pressure=Pideal=%fatm',Pideal);
f=p1^2/Pideal;
printf('\nFugacity of the N2gas=f=%fatm',f);
```

Scilab code Exa 5.34 Standard Entropy change

```
M=18;//molecular weight of water in grams//
Dl=0.958;//density of water in liquid form in gram
   per cm^3//
Dv=5.98*10^-4;//density of water in vapour form in
   gram per cm^3//
MVl=M/Dl;//molar volume of water in liquid form in
   cm^3//
MVv=M/Dv;//molar volume of water in vapour form in
   cm^3//
L=540;//Latent heat of vapourization in cal per gram
   //
T=373;//temperature in kelvin//
dV=30.11;
dP=(L*M)/(T*dV);
```

```
10 printf('dP/dT=0.357atm per deg=28.55mm of Hg per deg
   ');
11 dS=dP*dV;//change in entropy in cal per deg per mol
   //
12 printf('\nChange in entropy=dS=%fcal per deg per mol
   ',dS);
```

Scilab code Exa 5.35 Vapour pressure

```
1 dS=21.0;//standard entropy change of benzene in cal
   per deg per mol//
2 Tb=353;//boiling point of benzene in kelvin//
3 Lv=dS*Tb;//latent heat of vapourization of benzene
   in cal per mol//
4 printf('Latent heat of vapourization of benzene=Lv=
   %fcal per mol',Lv);
5 T=300;//temperature in kelvin//
6 R=1.99;//universal gas constant//
7 P=10^(Lv*((1/Tb)-(1/T))/(2.303*R));//vapour pressure
    of benzene in atm//
8 PHg=P*760;//vapour pressure in mm of Hg//
9 printf('\nvapour pressure of benzene=P=%fatm',P);
10 printf('\nVapour pressure of benzene in mm of Hg=PHg
   =%fmm of Hg',PHg);
```

Scilab code Exa 5.36 Operating temperature

```
1 T2=373;//final temperature in kelvin//
2 Lv=540*18;//latent heat of vapourization of water in
    cal per mol//
3 P1=1/20;//initial pressure in atm//
4 P2=1;//final pressure in atm//
5 R=1.99;//universal gas constant//
```

```
6 T1=1/((1/T2)+(2.303*R*log10(P2/P1)/Lv));
7 printf('\noperating temperature of the reactor=T1=
    %fK',T1);
8 printf('\nHence the plant can be operated at a
    temperature of 303.500Kelvin or 30.500degrees \
    nsince at a temperature higher than this the
    liquid phase no longer exists.');
```

Scilab code Exa 5.37 Vapour pressure

```
1 T1=373;//initial temperature in kelvin//
2 Lv=540*18;//latent heat of vapourization of water in
    cal per mol//
3 T2=423;//final temperature in kelvin//
4 R=1.99;//universal gas constant//
5 P=10^(-Lv*((1/T2)-(1/T1))/(2.303*R));//vapour
    pressure of water in atm//
6 printf('\npressure of water at which we can produce
    superheated steam=P=%fatm',P);
```

Scilab code Exa 5.38 Standard free energy change

```
1 PPSO3=1;//partial pressure of SO3 in atm//
2 PPSO2=0.2;//partial pressure of SO2 in atm//
3 PPO2=0.05;//partial pressure of O2 in atm//
4 Kp=3.5;
5 R=0.0821;//universal gas constant//
6 T=1000;//temperture in kelvin//
7 n1=3;
8 n2=2;
9 dn=n2-n1;//change in no. of moles//
10 Kc=Kp/((R*T)^dn);
11 printf('Kc for the reaction=Kc=%flitre per mol',Kc);
```

```
12 P=2;//pressure in atm//
13 Kinfinite=Kp/(P^dn);
14 printf('\nKinfinite of the reaction=Kinfinite=%fper
      atm',Kinfinite);
15 Qp=(PPSO3^2)/(PPSO2^2*PPO2);//reation quotient
      involving pressures//
16 printf('\nReaction quotient invloving pressures=Qp=
      %f',Qp);
17 dGO=-2.303*1.99*10^-3*T*log10(Kp);
18 printf('\ndGO=%f',dGO);
19 dG=dGO+(2.303*1.99*10^-3*T*log10(Qp));
20 printf('\nstandard free energy change in the
      reaction at 1000k=dG=%fKcal',dG);
21 printf('\nIt must be noted that under these
      conditions dG is positive.\nso it is the
      dissociation of SO3 that is spontaneous.');//here
       the answer given in the textbook is wrong the
      right one is that we got here through execution//
```

Scilab code Exa 5.39 Composition of water gas

```
1 Kp=1.60;//Kp for water at equilibrium//
2 Kc=1.60;//at equilibrium Kp=Kc//
3 x=0.56;
4 printf('Kp=Kc=x^2/(1-x)^2=1.60\nUpon solving above
      equation we get x=0.56\nTotal no. of moles=1-x+1-
      x+x+x=2\nmole percent of CO=mole percent of H2O
      =0.56*50=28');
5 printf('\nmole percent of CO2=mole percent of H2
      =0.44*50=22\nSo 100 volumes of the mixture will
      contain 28volumes of CO,28volumes of H2O\
      n22volumes of CO2 and 22volumes of H2.');
```

Scilab code Exa 5.40 Enthalpy change

```
T1=1000;//initial temperature in kelvin//
Kp1=0.72;//Kp value at T1 temperature//
T2=1260;//final temperature in kelvin//
Kp2=1.60;//Kp value at T2 temperature//
R=1.99;//universal gas constant//
printf('Since Kp2>Kp1 one would expect dH to be
    positive i.e Endothermic reaction.');
dH=(2.303*R*T1*T2*log10(Kp2/Kp1))/(T2-T1);
printf('\ndH for the reaction=dH=%fcal=7.702Kcal',dH
    );
```

Scilab code Exa 5.41 value of Kp

```
P=10;//pressure in atm//
printf('The total pressure P=PH2+PN2+PNH3.At all
    times PH2=3PN2\nSo PNH3=P-4*PN2 or PN2=0.25*(P-
    PNH3).');
printf('\nLet x represent the mole fraction of NH3
    at equilibrium.\nThen 1-x represents the sum of
    the mole fraction of N2 and H2.');
x=0.0122;//yield of NH3 in moles//
PNH3=x*P;//pressure of NH3 in atm//
xNH3=x;
PN2=0.25*(1-x)*P;//pressure of N2 in atm//
PH2=0.75*(1-x)*P;//pressure of H2 in atm//
Kp=(PNH3^2)/(PN2*PH2^3);
printf('\nKp value for the reaction=Kp=%f=1.5*10^-5
    atm^-2',Kp);
```

Scilab code Exa 5.42 Vapour pressure

```
printf('If the yield of NH3 is 12.2mol percent,x
   =0.122');
x=0.122;//yield of NH3 in moles//
Kp=1.48*10^-5;//Kp value of the equation in atm^-2//
P=sqrt((256*x^2)/(27*Kp*(1-x)^4));//pressure of the
   system in atm//
printf('\nPressure of the system=P=%fatm',P);
```

Scilab code Exa 5.44 Dissociation constant

```
printf('PCl5=PCl3+Cl2');
M0=208.5;
P=1;//pressure in atm//
w=4.59;//weight of PCl5 in grams//
V=1.7;//volume of PCl5 in gm^3//
T=523;//temperature in kelvin//
R=0.0821;//universal gas constant//
M=(w*R*T)/(P*V);
printf('\nMolecular weight of PCl5=M=%f',M);
a=(M0-M)/(M*(2-1));
printf('\na=%f',a);
Kp=(a^2*P)/(1-a^2);
printf('\nKp for the reaction=Kp=%f',Kp);
printf('\nIf total pressure is increased at the same
    temperature,Kp being constant,a should decrease
   .\nLet the degree of dissociation when P=2atm be
   a1 at the same temperature.');
P1=2;
a1=sqrt(Kp/(P1+Kp));
printf('\na1=%f',a1);//the answers in textbook are
   slightly different from what we got here but it's
    nothing wrong//
```

Scilab code Exa 5.45 Total pressure

```
a=0.5;//dissociation constant//
Kp=(a^2*P)/(1-a^2);
printf('Total pressure required to bring 50percent
   dissociation=P=3*Kp');
```

Scilab code Exa 5.46 Dissociation constant

```
a=0.21;//dissociation constant//
P=1;//pressure in atm//
Kp=(a^2*P)/(1-a^2);
printf('\nKp for the reaction=Kp=%f',Kp);
printf('\nP=1atm=0.4+PCOCl2+PCO+PCl2\nsum of
   pressure reactants=0.6atm\nCOCl2=CO+Cl2\nHere P
   is the total pressure due to all the participants
    of the reaction and is equal to 0.6atm.');
P1=0.6;
a1=sqrt(Kp/(P1+Kp));
printf('\na1=%f',a1);
printf('\nfor Pressure of 0.6atm a has increased,
   thereby indicating that the forward reaction is
   favoured.');//here the value of a1 is slightly
   different from textbook//
```

Scilab code Exa 5.47 Formation of ester

```
acid=1/3;
ester=2/3;
alcohol=1/3;
water=2/3;
K=(ester*water)/(acid*alcohol);
printf('K value of the reaction=K=%f',K);
```

```
7 printf('\nIn finding no. of moles we end up with
    quadratic equation 3*x^2-24*x+20=0.\nupon solving
     the equation we get x=7.05 and 0.945.');
8 printf('\nThe first solution is not admissible since
     the maximum yield of the ester cannot exceed one
     mol of acetic acid.\nHence x=0.945 i.e yield of
    the ester is 94.5percent.');
9 printf('\nThis problem illustrates the influence of
    an increased concentration of the reactant\nSince
     using one mole of each reactant the yield of
    ester is only 66.66percent');
10 acid=1-x;
11 ester=x;
12 alcohol=1-x;
13 water=1+x;
14 printf('\nIn finding no. of moles we end up with
    quadratic equation 3*x^2-9*x+4=0.\nupon solving
    the equation we get x=2.457 and 0.5425.');
15 printf('\nThe first solution is not admissible,x
    =0.5425.\nyield of the ester in the presence of
    the product water has decreased from 66.67percent
     to 54.25percent.');
16 printf('\nother homogeneous equilibria in the liquid
     phase such as ionization of weak acids\
    nionization of weak bases,hydrolysis of salts,etc
    .,can be treated likewise.');
```

Scilab code Exa 5.48 Equilibrium constant

```
1 Kp=29.64;//dissociation pressure of CaCO3 in mm of
    Hg//
2 printf('CaCO3+C=CaO+2CO for the dissociation of
    CaCO3=CaO+CO2');
3 printf('\nKp1=PCO2=29.64/760=0.039atm\nFor the
    reduction of CO2 by C,CO2+C=2CO.Kp2=PCO^2/PCO2\
```

```
    nVolume percent=mol percent=mole fraction*100\
    nPCO=xCO*total pressure=xCO since total pressure
    =1atm\nxCO=PCO=0.724atm and xCO2=PCO2=0.276atm');
printf('\nKp2=PCO^2/PCO2=(0.724)^2/0.276=1.9atm');
Kp1=0.039;//dissociation pressure of CaCO3 in atm//
Kp2=1.9;
Kp3=Kp1*Kp2;//equilibrium constant for overall
    reaction in atm^2//
printf('\nEquilibrium constant for overall reaction=
    Kp3=%f=7.41*10^-2atm^2',Kp3);
```

Scilab code Exa 5.49 Molecular weight

```
MH2O=18;//Molecular weight of H2O in grams//
WH2O=100;//weight of H2O in grams//
W=3.6;//weight of oraganic substance in grams//
dP=0.0855;//Lowering in vapour pressure in mm of Hg
    //
P=23.76;//Vapour pressure of Organic substance in mm
     of Hg//
M=(W*MH2O*P)/(WH2O*dP);//Molecular weight of Organic
     substance in grams//
printf('Molecular weight of Organic substance=M=
    %fgrams',M);
```

Scilab code Exa 5.50 Molecular weight

```
T0=373;//temperature in kelvin//
R=1.99;//value of R in cal per deg per mol//
lv=540;//Latent heat of vaporization in cal per
    grams//
Kb=(R*T0^2)/(1000*lv);//value of Kb in deg per mol//
printf('Value of Kb=%fKbdeg per mol',Kb);
```

```
6  T1=373.57;//temperature in kelvin//
7  W2=5;//weight of urea in grams//
8  W1=75;//weight of water boils in grams//
9  dT=T1-T0;//change in temperature//
10 M2=(Kb*1000*W2)/(dT*W1);//Molecular weight of urea
       in grams//
11 printf('\nMolecular weight of urea=M2=%fgrams',M2);
```

Scilab code Exa 5.51 Freezing point

```
1  lf=80;//Latent heat of fusion of Ice in cal per gram
       //
2  lv=540;//Latent heat of evaporation of water in cal
       per gram//
3  Tf=273;//fusion temperature in kelvin//
4  Tb=373;//Boiling temperature in kelvin//
5  dTb=Tb-Tf;//change in temperature//
6  dTf=(dTb*Tf^2*lv)/(Tb^2*lf*1000);
7  FP=0-dTf;//Freezing point of the solution//
8  printf('The Freezing point of the solution=FP=%f',FP
       );
```

Scilab code Exa 5.52 Quantity of methanol and ethylene

```
1  Kf=1.86;//Kf for water//
2  M2=32;//Molecular weight of Methanol in grams//
3  W1=10000;//weight of H2O in grams//
4  dTf=10;//lowering freezing point of water//
5  W2=(dTf*W1*M2)/(1000*Kf);//weight of methanol in
       grams//
6  printf('weight of Methanol=W2=%fgrams=1.72Kg',W2);
7  M3=62;//Molecular weight of Ethylene in grams//
```

```
8 W3=(dTf*W1*M3)/(1000*Kf);//weight of methanol in
    grams//
9 printf('\nweight of Ethylene=W3=%fgrams=3.334Kg',W3)
    ;
```

Scilab code Exa 5.53 Quantity of ice

```
1 Kf=1.86;//Kf for water//
2 printf('At -18.6degrees temperature only Ice
    seperates from the Aqueous solution\nThe weight
    of Glycol remains constant through its
    concentration Actually increases since ice
    seperates out on cooling.');
3 printf('\nInitial Concentration=3334grams per 10Kg
    of Water.');
4 dT=18.6;
5 m=dT/Kf;
6 w=10;//initial content of water in litres//
7 w1=5.376;
8 W=w-w1;//weight of ice seperating in kilograms
9 printf('\nIf dT=18.6 then m=10');
10 printf('\nAt -18.6Degrees 10 mol of glycol are
    present in 1000grams of water,i.e 620grams in
    1000grams of water,or 6200grams in 10Kg of water.
    ');
11 printf('\n3334grams of glycol would be present in
    10*3334/6200,i.e 5.376Kg of Water.');
12 printf('\nWt. of Ice seperating=W=%fKg',W);
```

Scilab code Exa 5.54 Osmotic pressure

```
1 T=300;//temperature in kelvin//
2 R=0.0821;//universal gas constant//
```

```
3 Ws=0.171;//Weight of Sucrose  in the solution in
    grams//
4 Ms=342;//Molecular weight of Sucrose in grams//
5 l=0.05;//volume of solution in litres//
6 ns=(Ws)/(Ms*l);//no. of moles of sucrose in the
    solution//
7 printf('Osmatic pressure being a colligative
    property depends only on the no. of mol of solute
     present and not on their nature.');
8 printf('\nNo. of moles of Sucrose in a litre
    solution=ns=%fmol per litre',ns);
9 Wg=0.18;//Weight of glucose  in the solution in
    grams//
10 Mg=180;//Molecular weight of glucose in grams//
11 ng=(Wg)/(Mg*l);//no. of moles of glucose in the
    solution//
12 printf('\nNo. of moles of Glucose in a litre
    solution=ns=%fmol per litre',ng);
13 Wu=0.06;//Weight of Urea in the solution in grams//
14 Mu=60;//Molecular weight of Urea in grams//
15 nu=(Wu)/(Mu*l);//no. of moles of Urea in the
    solution//
16 printf('\nNo. of moles of Urea in a litre solution=
    ns=%fmol per litre',nu);
17 c=ns+ng+nu;//total no of moles in a litre solution//
18 printf('\nTotal no. of moles in a litre solution=c=
    %fmol per litre',c);
19 OP=c*R*T;//Osmatic pressure in atms//
20 printf('\nOsmatic pressure of the solution at 300k=
    OP=%fatm',OP);
```

Scilab code Exa 5.55 Molecular weight

```
1 Hb=2.4;//rise of the benzene solution in mm//
2 Db=0.88;//Density of Benzene solution in g per cm
```

```
    ^3//
Dm=13.6;//Density of mercury solution in g per cm
    ^3//
Hm=(Hb*Db)/Dm;//Rise of mercury solution in mm//
printf('The Osmatic pressure given in terms of the
    height of a liquid column must be converted into
    an equivalent height of a mercury column.');
printf('\nEquivalent Height of the mercury column=Hm
    =%fmm',Hm);
printf('\nThe density of solution is equal to
    density of solvent since the solution is dilute.\
    nLet M2 be the molecular weight of polymer.');
R=0.0821;//Universal gas constant//
T=310;//temperature in kelvin//
M2=(2.5*R*T*760)/Hm;//Molecular weight of polymer in
    grams//
printf('\nMolecular weight of polymer=M2=%f
    =3.11*10^5grams',M2);
```

Scilab code Exa 5.56 Concentration of glucose

```
T=310;//temperature in kelvin//
R=0.0821;//universal gas constant//
OP=7.65;//Osmatic pressure in atm//
c=OP/(R*T);
printf('Concentration of glucose=c=%fM',c);
W=c*180;//weight in one litre in grams//
printf('\nWeight in one litre=W=%fgrams',W);
```

Scilab code Exa 5.57 degree of dissociation

```
T0=373;//temperature in kelvin//
Kb=0.52;//value of Kb in deg per mol//
```

```
T1=373.208;//temperature in kelvin//
W2=3.40;//weight of BaCl2 in grams//
W1=100;//weight of water boils in grams//
dTb=T1-T0;//change in temperature//
Mobs=(Kb*1000*W2)/(dTb*W1);//Molecular weight of
   BaCl2 observed in grams//
printf('Molecular weight of BaCl2 observed=Mobs=
   %fgrams',Mobs);
Mthr=208.4;//Theoritical Molecular weight of BaCl2
   in grams//
i=Mthr/Mobs;
a=0.5*(i-1);//apparent degree of dissociation of
   BaCl2//
printf('\nApparent degree of dissociation of BaCl2=a
   =%f',a);
```

Scilab code Exa 5.58 Nature of the species

```
Kf=1.86;//Kf for water//
m=0.1;//no. of moles of organic mono carboxilic acid
   //
dTf=Kf*m;//Theoritical change in temperature//
printf('Theoritical change in temperature=dTf=%f',
   dTf);
dTobs=0.220;//Observed change in temperature//
i=dTobs/dTf;
printf('\nSince dTobs is greater than dTf ionization
    must have occurred in aqueous solution.\nAn
   organic monobasic acid RCOOH ionizes as RCOOH =
   RCOO- + H+.');
a=i-1;//degree of ionization//
printf('\nDegree of ionization=a=%f',a);
printf('\nIf the acid dissolved as such in its
   molecular form as species dTthr=5.12*0.1=0.512,
   dTobs=0.265.');
```

```
11 printf('\nThis value is nearly half the expected
      value,suggesting that the molecule exists as
      associated molecules in solution.');
12 i1=0.265/0.512;
13 a1=2*(1-i1);
14 printf('\nThe acid is demerized to the extent of a1
      =96.500000percent.')
```

Chapter 6

PHASE EQUILIBRIA

Scilab code Exa 6.1 Normality of solution

```
1 MW=249.6;//molecular weight of CuSO4.5H2O in grams//
2 w=0.3120;//weight of CuSO4.5H2O in grams//
3 V=0.25;//volume of the solution in litres//
4 printf('From Equation (a) 2 mol of CuSO4.5H2O
    liberates 1 mol of I2,i.e. 2 equivalents.\nHence
    the equlivalent weight of CuSO4.5H2O=mol.wt/1.');
5 printf('\nFrom equation (b) the equivalent weight of
     CuSO4.5H2O is mol.wt/2 since 1mol of CuSO4.5H2O
    reacts with 2 mol of OH-,i.e 2 equivalents.');
6 W=w/V;//weight of CuSO4.5H2O in one litre solution
    in grams//
7 printf('\nWeight of CuSO4.5H2O in a litre of the
    solution=W=%fgrams.',W);
8 Na=W/MW;//Normality of the solution for (a)//
9 printf('\nNormality of the solution for (a)=Na=%f',
    Na);
10 Nb=W*2/MW;//Normality of the solution for (b)//
11 printf('\nNormality of the solution for (b)=Nb=%f',
    Nb);
12 printf('\nIn the first case 1ml of the solution
    contains 5*10^-3equivalents or 5 equivalents of
```

```
CuSO4.5H2O,\nand in the second case 1ml of the
solution will contain 10m eq of CuSO4.5H2O.');
```

Scilab code Exa 6.2 Molality and mole fraction

```
1  v=180;//volume of conc. H2SO4 in ml//
2  n=6.61;//Normality of the solution//
3  N=1000*n/v;
4  printf('The Noramality or Strength of the Conc. acid
   =N=%fN',N);
5  printf('\n1 eq.per litre=0.5mol per litre in the
   case of H2SO4 since the eq.wt=0.5 the mol.wt.');
6  printf('\n 6.6N soln=6.61 eq per litre=3.305mol per
   litre.\n Strength of the diluted solution=3.305M'
   );
7  SG=1.84;//super gravity of Conc. H2SO4//
8  w=SG*v;//weight of 180ml of conc. H2SO4 in grams//
9  printf('\nWt of 180ml of conc.H2SO4=w=%fgrams.',w);
10 printf('\nThis actually contains 6.61*49grams of
   H2SO4.\n percentage of H2SO4 by weight=97.8');
11 sg=1.198;//specific gravity of the diluted solution
   //
12 V=1000;//volume of the diluted solution in ml//
13 W=sg*V;//weight of one litre of the diluted solution
    in grams//
14 printf('\nWt of 1 litre of the diluted solution=W=
   %fgrams ',W);
15 WH2O=w+W;//weight of water in grams//
16 printf('\ntherefore Weight of water=WH2O=%fgrams.',
   WH2O);
17 printf('\nIf the percent of H2SO4 by wt in the
   diluted solution is y.\nWt of H2SO4 in 1litre of
   the diluted solution=49*6.61grams.so y value
   comes as 27.04percent');
18 M=3.305*1000/WH2O;//molality of the solution//
```

```
19 printf('\nMolality of the solution=M=%f',M);
20 mf=0.064;//mole fraction of H2SO4//
21 mfH2O=1-mf;//mole fraction of water//
22 printf('\nMol of sulphuric acid is 329.9/98=3.305.\
     nMol of water=874.1/18=48.561.\nMol fraction of
     H2SO4=0.064.');
23 printf('\nMole fraction of water=mfH2O=%f',mfH2O);
```

Scilab code Exa 6.3 Percentage by weight

```
1 N2=79.2;//percentage of Nitrogen in air//
2 O2=20.8;//percentage of Oxygen in air//
3 b=76.93;//Weight percent of N2 in air//
4 printf('Weight percent of N2 in air=b=%f',b);
5 a=100-b;//weight percent of O2 in air//
6 printf('\nWeight percent of O2 in air=a=%f',a);
```

Scilab code Exa 6.4 Percentage of volume

```
1 N2=0.79;//partial pressure of Nitrogen in air//
2 O2=0.21;//partial pressure of Oxygen in air//
3 AN2=0.015;//Absorption coefficient of N2//
4 AO2=0.028;//Absorption coefficient of O2//
5 l=22.4;
6 printf('Absorption coefficient being the solubility
     of the gas at partial pressure of 1atm of the gas
     ,\nThe solubilities in mol per litre of the two
     gases are');
7 SN2=N2*AN2/l;//solubility of N2//
8 SO2=O2*AO2/l;//solubility of O2//
9 printf('\nSolubility of N2=SN2=%f=5.29*10^-4mol per
     litre.',SN2);
```

```
10 printf('\nSolubility of O2=SO2=%f=2.625*10^-4mol per
       litre',SO2);
11 VO2=(SO2*100)/(SN2+SO2);
12 printf('\nThe mole or Volume percent of O2=%f',VO2);
13 VN2=100-VO2;
14 printf('\nThe mole or volume percent of N2=%f',VN2);
```

Scilab code Exa 6.5 Vapour pressure

```
1 printf('Upon solving the equations PA=0.9atm,PB=0.3
     atm');
2 PA=0.9;//vapour pressure of A//
3 PB=0.3;//Vapour pressure of B//
4 xA=0.33;
5 xB=0.66;
6 yA=(xA*PA)/(xA*PA+xB*PB);
7 printf('\nComposition of Vapour A in the mixture=yA=
     %f',yA);
8 yB=1-yA;
9 printf('\nComposition of Vapour B in the mixture=yB=
     %f',yB);
10 VP=yA*PA+yB*PB;//total vapour pressure of the
     mixture//
11 printf('\nTotal vapour pressure of the mixture=VP=%f
     ',VP);
```

Scilab code Exa 6.6 Vapour pressure

```
1 yA=0.60;
2 xA1=0.40;
3 xA=0.5*yA+0.5*xA1;
4 printf('Let PA and PB represent the vapour pressures
     of pure A and pure B respectively.');
```

```
5 printf('\nFrom 1 mol of solution after distillation,
    we get 0.5mol of distillate and 0.5mol of residue
    .');
6 printf('\nVapour pressure of substance A=PA
    =900.00000mm of Hg');
7 printf('\nVapour pressure of substance B=PB
    =400.00000mm of Hg');
```

Scilab code Exa 6.7 Molecular weight

```
1 wA=162;
2 wB=100;
3 VPB=641;//vapour pressure of water//
4 VPA=119;//vapour pressure of oraganic substance//
5 MB=18;//Molecular weight of H2O//
6 printf('Even though the boiling part of A might be
    higher,it distills out at a low temperature 95.3
    degrees.');
7 printf('\nIf A were to distill at 95.3degrees,the
    distillation will have to be carried out at a
    reduced pressure of about 119mm of mercury');
8 MA=(wA*MB*VPB)/(wB*VPA);
9 printf('\nMolecular weight of A=MA=%fgrams',MA);
```

Scilab code Exa 6.8 Efficiency comparison

```
1 w=50;//weight of acid A in grams//
2 x=1;
3 y=0.2;
4 K=5;
5 n=5;
6 wn=w*(x/(x+K*y))^n;
7 printf('wn=%fgrams',wn);
```

```
y1=1;
w0=w*(x/(x+K*y1));
printf('\nw0=%fgrams',w0);
printf('\nIt is seen that the first process leaves
   only 1.563grams of A with the aq. layer,\nwhereas
    the secondone using all available solvent in a
   single lot leaves 8.333grams in aqueous layer.\
   nIn the process (a)96.88percent of A is extracted
   ,whereas in (b) only 83.67percent A is extracted.
   ');
```

Scilab code Exa 6.9 Neutralisation

```
AN=0.096;//normality of H2SO4 in aqua layer//
ON=0.014;//normality of H2SO4 in org. layer//
AV=13.3;//amount of H2SO4 required in aq. layer for
   neutralization//
OV=7.15;//amount of H2SO4 requred in org. layer for
   neutralization//
AS=AN*AV/10;//strength of NH3 in aq. layer//
printf('Strength of NH3 in aq. layer=AS=%fN.',AS);
OS=ON*OV/20;//strength of NH3 in org. layer//
printf('\nStrength of NH3 in org. layer=OS=%fN.',OS)
   ;
K=AS/OS;//equilibrium constant//
printf('\nEquilibrium constant=K=%f',K);
AV1=20.0;//amount of H2SO4 required in aq. layer at
   equilibrium//
OV1=8.0;//amount of H2SO4 required in org. layer at
   equilibrium//
AN1=AV1*AN/5;//Normality of NH3 in aq. layer//
printf('\nNormality of NH3 in aq. layer=AN1=%fN.',
   AN1);
ON1=OV1*ON/10;//Normality of NH3 in org. layer//
printf('\nNormality of NH3 in org. layer=ON1=%fN.',
```

```
    ON1);
17 printf('\nIn the aq.layer NH3 includes the free
    ammonia(uncombined).\nNH3t and that which has
    combined with Cu2+ to form the complex ion NH3.')
    ;
18 printf('\nNH3aq=NH3t+NH3combined.\nThe value of NH3t
     can be obtained from the value of K.\nK=25.49=
    NH3t/NH3combined.');
19 NH3t=K*ON1;
20 printf('\nSince nernsts law holds good for the same
    species present in both phases.\nNH3t=%f=0.2855N.
    ',NH3t);
21 NH3c=AN1-NH3t
22 printf('\nNH3c=%f=0.0985N',NH3c);
23 printf('\n0.025mol per litre of Cu2+ combines with
    0.0985mol per litre of NH3.\n1 mol per litre of
    Cu2+ combines with 0.0985/0.025=3.936mol per
    litre of NH3.');
24 printf('\nor 1mol of Cu2+ combines with 4mol of NH3,
    i.e the value of x is 4.\nThe formula of the
    complex ion is thus (Cu(NH3)4)2+');
```

Chapter 7

ELECTROCHEMISTRY

Scilab code Exa 7.1 Number of electrons per second

```
1 q=4.0*10^-3;//quantity of electricity in coulombs//
2 e=1.6*10^-19;//charge of an electron in coulombs//
3 N=q/e;//no. of electrons per second//
4 printf('No. of electrons per second=N=%f=2.5*10^16',
    N);
```

Scilab code Exa 7.2 Thickness of the deposit

```
1 i=3;//current passed through the solution in amps//
2 t=5;//amount of time current passed through in hours
    //
3 q=(i*t)/26.8;//quantity of electricity passed in
    farads//
4 printf('Quantity of electricity passed=q=%fFarads',q
    );
5 printf('\nIf all the current is used in the
    deposition of Ni,i.e 100percent efficiency 0.56
    equivalents of Ni should be deposited at the
    cathode.');
```

```
N=0.56*0.60;//No. of equivalents of Ni deposited//
printf('\nNo. of equivalents of Ni deposited=N=%f',N
   );
w=58.71;//weight of Ni in grams//
wd=N*w/2;//weight of Ni actually deposited in grams
   //
printf('\nWeight of Ni actually deposited=wd=%fgrams
   ',wd);
TA=32;//total area of the cathode in cm^2 for 2faces
   //
d=8.9;//density of Ni in gram per cm^3//
V=wd/d;//volume of the Ni deposited in cm^3//
printf('\nVolume of the Ni deposited=V=%fcm^3',V);
T=V/TA;//thickness of the deposit in cm//
printf('\nThickness of the deposit=T=%fcm',T);
printf('\nOut of 0.56Farad, 0.336Farad is used for
   Ni deposition\nhence 0.224Farad is used for
   liberation of hydrogen.');
printf('\n0.224 equivalent of hydrogen is
   =11.2*0.224=2.51litres.');
```

Scilab code Exa 7.3 time of current supply

```
i=5*10^-3;//steady current given by the cell in amps
   //
w=1.7399;//amount of MnO2 used in grams//
MW=86.95;//molecular weight of MnO2 in grams//
F=96500;//farad value in coulombs//
C=0.02*F;//charge value in coulombs//
printf('From the cathode reaction 2mol of MnO2=2
   Farad.');
printf('\n0.02Farad means  the charge=C=%fCoulombs.'
   ,C);
q=1930;//charge in coloumbs corresponding to 0.02
   Farad//
```

```
t=q/i;//amount of time cell suplies the current in
    seconds//
printf('\nAmount of time cell supplies the current=t
    =%f=3.86*10^5seconds',t);
```

Scilab code Exa 7.4 Cell constant and equivalent conductance

```
C=2.768*10^-3;//conductivity of the cell in ohm^-1
    cm^-1//
R=82.4;//resistance with KCl solution filled in ohms
    //
K=C*R;//cell constant in cm^-1//
printf('Cell constant=K=%fcm^-1',K);
R1=326;//resistance with K2SO4 solution filled in
    ohms//
c=K/R1;//Equivalent conductance of the KCl solution
    in ohm^-1 cm^-1//
printf('\nEquivalent conductance of the KCl solution
    =c=%f=7*10^-4ohm^-1 cm^-1',c);
printf('\n0.0025M K2SO4 solution=0.005N of K2SO4.');
EC=1000*c/0.005;//equivalent conductance of K2SO4
    solution in ohm^-1 cm^2//
printf('\nEquivalent conductance of K2SO4 solution=
    EC=%fohm^-1cm^2',EC);
```

Scilab code Exa 7.5 Transport number

```
wAg=1.424;//weight of Ag deposited in the coulometer
    in grams//
MW=108;//molecular weight of AgNO3 in grams//
w1=90.25;//weight of silver nitrate in grams//
w2=5.039;//weight of AgNO3 in grams//
w=w1-w2;
```

```
6 n=wAg/MW;
7 printf('No. of equivalents of Ag deposited in the
    silver coulometer=n=%f.',n);
8 printf('\nThis amount of Ag+ and NO3- ions would
    have discharged at the cathode and at the anode
    respectively.');
9 printf('\n Anolyte solution\nBefore electrolysis
    85.21(90.25-5.039)grams of water contained
    0.02965 equivalents of AgNO3 or Ag+.');
10 BEAg=0.007202;//no. of equivalents of Ag+ before
    electrolysis//
11 printf('\nAfter electrolysis 20.893-0.193 i.e 20.7
    grams of water contains 0.001136equivalents of
    AgNO3 or Ag+.');
12 AEAg=0.01136;//no. of equivalents of Ag+ after
    electrolysis//
13 printf('\n20.7grams of water,before electrolysis
    would have contained 0.007202 equivalents of Ag+.
    ');
14 DC=BEAg-AEAg;//decrease in the conc. of anolyte//
15 printf('\nDecrease in the conc. of anolyte=DC
    =0.006066equivalents.');
16 tAg=n/DC;//transport number//
17 printf('\ntAg=ratio of Decrease in anolyte conc. and
     No. of gram equivalents deposited at either
    electrode=tAg=0.460100');
```

Scilab code Exa 7.6 Transport number

```
1 wCu=0.0230;//weight of Cu deposited in the
    coulometer in grams//
2 MW=63.54;//molecular weight of Cu in grams//
3 n=wCu*2/MW;//no. of equivalents of Cu deposited//
4 printf('In the coulometer,wt of Cu deposited=0.0230
    grams');
```

```
5  printf('\nNumber of equivalents of Cu deposited=n=
       %fequivalents or Farads.',n);
6  printf('\nThis would have resulted in deposition of
       7.24*10^-4equivalents of Ag+ at the cathode \nand
        dissolution of the same amount at the anode.');
7  wAgNO3=7.39;
8  w1AgNO3=0.2360;//after electrolysis weight of AgNO3
       //
9  MWAgNO3=170;//molecular weight of AgNO3//
10 BEAgNO3=wAgNO3/MWAgNO3;
11 printf('\n Anolyte solution \nBefore electrolysis
       1000grams of water contains %fequivalents of
       AgNO3',BEAgNO3);
12 AEAgNO3=w1AgNO3/MWAgNO3;
13 printf('\nAfter electrolysis 23.14grams of water
       contains %fequivalents of AgNO3.',AEAgNO3);
14 w=23.14;
15 BE=w*BEAgNO3/1000;
16 printf('\n23.14grams of water before electrolysis
       would have contained %fequivalents of AgNO3',BE);
17 IC=AEAgNO3-BE;
18 printf('\nIncrease in the concentration of anolyte=
       IC=%fequivalents.',IC);
19 printf('\n0.000382gram equivalents of NO3- ions must
        have migrated into the anode compartment.\nAs a
       result of passin 7.24*10^-4Farads into the
       solution.\n0.000724equivalents of Ag should have
       dissolved to give the same amount of Ag+ ion.\
       nOut of this 0.000382gram equivalents are present
        in the anolyte.');
20 ME=n-IC;//no of equivalents of migrated anodes//
21 printf('\n%fgram equivalents of Ag+ ions must have
       migrated from the anode.',ME);
22 tAg=ME/n;//transport number//
23 printf('\nTransport number of Ag=tAg=%f',tAg);
24 tSO3=1-tAg;
25 printf('\nTransport number of SO3=tSO3=%f',tSO3);
```

Scilab code Exa 7.7 Ionic conductances and ionic mobilities

```
EC=426;//equivalent conductance of HCl in ohm^-1cm^2//
tH=0.82;//transport number of H+//
tCl=0.18;//transport number of Cl-//
ICH=EC*tH;//ionic conductance of H+ in ohm^-1cm^2//
printf('Ionic conductance of H+=ICH=%fohm^-1cm^2',ICH);
ICCl=EC*tCl;//ionic conductance of Cl- in ohm^-1cm^2//
printf('\nIonic conductance of Cl-=ICCl=%fohm^-1cm^2',ICCl);
F=96500;
IMH=ICH/F;//ionic mobility of H+ in cm^2v^-1s^-1
printf('\nIonic mobility of H+=IMH=%f=36.20*10^-4cm^2v^-1s^-1',IMH);
IMCl=ICCl/F;//ionic mobility of H+ in cm^2v^-1s^-1
printf('\nIonic mobility of H+=IMCl=%f=7.95*10^-4cm^2v^-1s^-1',IMCl);
```

Scilab code Exa 7.9 degree of dissociation and Ionization constant

```
printf('A solution of NH3 is alkaline due to the following hydrolysis\nNH3+H2O = NH4+ + OH-');
printf('\nKb=(NH4+)*(OH-)/(NH3)=(c*a^2)/(1-a). ');
EC=3.7;//equivalent conductance of NH3 in water in ohm^-1cm^2//
EC0NH4Cl=149.9;//equivalent conductance of NH4Cl in ohm^-1cm^2//
EC0BaCl2=139.9;//equivalent conductance of 1/2BaCl2 in ohm^-1cm^2//
```

```
6 EC0BaOH2=262.2;//equivalent conductance of 1/2Ba(OH)
    2 in ohm^-1cm^2//
7 EC0=EC0NH4Cl-EC0BaCl2+EC0BaOH2;//effective
    Equivalent conductance in ohm^-1cm^2//
8 printf('\nEC0=%fohm^-1cm^2',EC0);
9 a=EC/EC0;//dissociation constant of the solution//
10 printf('\nDissociation constant of the solution=a=%f
    ',a);
11 C=0.1;//normality of the solution//
12 Kb=(C*a^2)/(1-a);
13 printf('\nIonization constant=Kb=%f',Kb);//here the
    values of a and Kb are slightly different from
    textbook but that is ok//
```

Scilab code Exa 7.10 Solubility of BaSO4

```
1 SCsat=4.63*10^-6;//Specific conductance of saturated
    solution in ohm^-1cm^-1//
2 SCused=1.12*10^-6;//specific conductance of the
    water used in the experiment//
3 SC0Na2SO4=130.1;//specific conductance of Na2SO4 in
    ohm^-1cm^-1//
4 SC0BaCl2=139.9;//specific conductance of 1/2BaCl2 in
    ohm^-1cm^-1//
5 SC0NaCl=126.5;//specific conductance of NaCl in ohm
    ^-1cm^-1//
6 SC0=SC0Na2SO4-SC0NaCl+SC0BaCl2;//effective specific
    conductance in ohm^-1cm^2//
7 printf('SC0=%fohm^-1cm^-1',SC0);
8 SC=SCsat-SCused;
9 printf('\nSpecific conductance of the experiment=SC=
    %f=3.51*10^-6ohm^-1cm^-1',SC);
10 S=(SC*1000)/SC0;//Solubility of the solution//
11 printf('\nSolubility of the solution=S=%f
    =2.437*10^-5gram equivalent per litre',S);
```

```
12 printf('\n1mol of BaSO4=2equivalents')
13 SBaSO4=S/2;//Solubility of the BaSO4 solution//
14 printf('\nSolubility of the BaSO4 solution=SBaSO4=%f
   =1.218*10^-5mol litre^-1',SBaSO4);
```

Scilab code Exa 7.11 Iconic strength

```
1 M1=0.1;//molarity of KCl//
2 IKCl=0.5*(M1*1^2+M1*1^2);//Iconic strength of KCl//
3 printf('Iconic strength of KCl=IKCl=%f',IKCl);
4 M2=0.2;//molarity of K2SO4//
5 IK2SO4=0.5*(2*M2*1^2+M2*2^2);//Iconic strength of
   K2SO4//
6 printf('\nIconic strength of K2SO4=IK2SO4=%f',IK2SO4
   );
7 M3=0.2;//molarity of MgCl2//
8 IMgCl2=0.5*(M3*2^2+2*M3*1^2);//Iconic strength of
   MgCl2//
9 printf('\nIconic strength of MgCl2=IMgCl2=%f',IMgCl2
   );
10 I=IKCl+IK2SO4+IMgCl2;//total iconic strength of the
   mixture//
11 printf('\nTotal Iconic strength of the mixture=I=%f'
   ,I);
```

Scilab code Exa 7.12 Maximum concentration

```
1 r=0.96;
2 I=(log10(r)/-0.51)^2;//Iconic strength of the HCl
   solution//
3 printf('Iconic strength of the HCl solution=I=%f',I)
   ;
4 printf('\nHCl being a 1,1 electrolyte I=c');
```

```
5 printf('\nSo the maximum concentration of HCl to be
    used=I=c=1.20*10^-3');
```

Scilab code Exa 7.13 Concentrations of ions

```
1 w=3.55;//weight of the salt in grams//
2 MW=258.2;//Molecular weight of the salt//
3 printf('KAl(SO4)2 = K+ + Al3+ + 2SO42-');
4 c=w*4/MW;//Concentration of the salt//
5 printf('\nConcentration of the salt=c=%fM',c);
6 SO4=2*c;//Concentration of SO42- in the solution//
7 printf('\nconcentration of K+ = Al3+ =%fM',c);
8 printf('\nConcentration of SO42- =%fM',SO4);
```

Scilab code Exa 7.14 Ionization strength

```
1 c=0.1;//concentration of the solution//
2 a=1.332*10^-2;//Ionization constant//
3 Ka=(c*a^2)/(1-a);
4 printf('CH3COOH = CH3COO- + H+');
5 printf('\nKa value for the reaction=Ka=%f
    =1.799*10^-5',Ka);
```

Scilab code Exa 7.15 Ionization strength

```
1 c=0.1;//concentration of the solution//
2 Kb=1.8*10^-5;
3 printf('The value of a should be calculated first
    using Kb=(c*a^2)/(1-a)\nThis gives rise to a
    quadratic equation which can be solved to obtain
    the value of a.');
```

```
4 printf('\nUsually it is permissible to use
    approximation methods if K<10^-5\nOne can neglect
     a in comparison to 1 and solve for a.\nA better
    way is to use the method of succesive
    approximations.\nThis will be illustrated using
    the above equation');
5 printf('\nFirst find the approximate value of a by
    neglecting the value of a in comparison with 1.\
    nLet the approximate value be a1');
6 a1=1.342*10^-2;
7 a2=1.332*10^-2;
8 printf('\nWe repeat this procedure till 2
    consecutive values of a do not differ
    significantly.');
9 a3=1.332*10^-2;
10 OH=a3*c;//concentration of OH- in the solution//
11 printf('\nSince the values of a2 and a3 are the same
     the correct value of a=1.332*10^-2\nThe
    approximate value is greater than the correct
    value by about 1percent.');
12 printf('\nThe concentration of OH- =%f=1.332*10^-3M'
    ,OH);
```

Scilab code Exa 7.18 Relative strengths

```
1 Kw=1.0^10^-14;
2 KH1=1.0*10^-5;//KH value of H+ ion in RCOOH//
3 KH2=1.0^10^-10;//KH value of H+ ion in HCN//
4 Kb1=Kw/KH1;//Kb value for RCOO- ion//
5 printf('Kb value for RCOO- ion=10^-9 ');
6 Kb2=Kw/KH2;//Kb value for CN- ion//
7 printf('\nKb value for CN- ion=10^-4');
8 printf('\nCN- is about 10^5 times stronger than RCOO
    - as a base.');
```

Scilab code Exa 7.19 PH of the solutions

```
c1=1;//concentration of HCl//
PH1=-log10(c1);
printf('PH for the 1M HCl solution=PH1=%f',PH1);
c2=5.2*10^-4;//concentration of H+ in the solution//
PH2=-log10(c2);
printf('\nPH for the solution=PH2=%f',PH2);
c3=0.025;//concentration of 0.025M HClO4//
PH3=-log10(c3);
printf('\nPH for the 0.025M HClO4 solution=PH3=%f',
   PH3);
PH4=4.45;
c4=10^(-PH4);//concentration of the solution//
printf('\nConcentration of the solution=c4=%f
   =3.548*10^-5',c4);
POH5=1.30;
PH5=14-POH5;
c5=10^(-PH5);//concentration of the solution//
printf('\nConcentration of the solution=c5
   =1.995*10^-13');
```

Scilab code Exa 7.20 PH and POH of the solutions

```
a=1.33*10^-2;//Ionization constant//
c=0.1;//concentration of the solution//
OH=a*c;
printf('OH- =a*c=1.33*10^-3');
POH=-log10(OH);//POH of the solution//
printf('\nPOH of the solution=POH=%f',POH);
PH=14-POH;//PH of the solution//
printf('\nPH of the solution=PH=%f',PH);
```

Scilab code Exa 7.21 PH of the solution

```
c=0.01;//concentration of the solution//
r=10^(-0.51*sqrt(c));
printf('r=%f',r);
a=r*c;//ionization constant//
printf('\nIonization constant=a=%f',a);
PH=-log10(a);//PH of the solution//
printf('\nPH of the solution=PH=%f',PH);
printf('\nBy assuming ideal behaviour PH=-log10
   (10^-2)=2.00');
```

Scilab code Exa 7.22 PH of a buffer solution

```
CNH3=0.1;//concentration of NH3 solution//
CNH4Cl=0.1;//concentration of NH4Cl solution//
POH=4.74;
PH=14-POH+log10(CNH3/CNH4Cl);
printf('PH of the solution=PH=%f',PH);
printf('\nOn adding 0.01mol of HCl,assuming that no
   volume change occurs,0.01mol of NH4Cl is produced
   .\nTherefore,the concentration of NH3 decreases
   by 0.01 and that of NH4Cl increases by 0.01 ');
C1NH3=0.09;
C1NH4Cl=0.11;
PH1=14-POH+log10(C1NH3/C1NH4Cl);
printf('\nPH of the solution=PH1=%f',PH1);
printf('\nOn adding 0.01mol of NaOH,assuming that no
    volume change occurs,0.01mol of NH3 is produced
   .\nTherefore,the concentration of NH3 increases
   by 0.01 and that of NH4Cl decreases by 0.01 ');
```

```
12 C2NH3=0.11;
13 C2NH4Cl=0.09;
14 PH2=14-POH+log10(C2NH3/C2NH4Cl);
15 printf('\nPH of the solution=PH2=%f',PH2);
```

Scilab code Exa 7.23 Hydrolysis constant and degree of hydrolysis

```
1  c=0.1;//concentration of the solution//
2  Kw=1.0*10^-14;
3  Ka=7.24*10^-10;//dissociation constant of HCN//
4  printf('For a salt of this type the hydrolysis
       reaction is\nCN- +H2O = HCN + OH-');
5  Kh=Kw/Ka;//hydrolysis constant//
6  printf('\nHydrolysis constant of the solution=Kh=%f
       =1.381*10^-5',Kh);
7  printf('\nIonization constant is generally
       calculated using  Kh=(c*a^2)/(1-a)');
8  printf('\nIonization constant=a=0.011680=1.168*10^-2
       ');
9  printf('\nThe degree of hydrolysis is 1.168percent')
       ;
10 PKw=23.14;
11 PH=0.5*(PKw+log10(c));//PH of the 0.1M NaCN solution
       //
12 printf('\nPH of the 0.1M NaCN solution=PH=%f',PH);
```

Scilab code Exa 7.25 Solubility

```
1 MW=332;//molecular weight of Ag2CrO4 in grams//
2 s=2.5*10^-2;//solubility of Ag2CrO4 in g per litre//
3 S=s/MW;//Solubility of Ag2CrO4 in mol per litre//
4 printf('Solubility of Ag2CrO4=S=%f=7.5*10^-5mol per
      litre',S);
```

```
5 Ag=2*7.5*10^-5;//Solubility of Ag component in mol
    per litre//
6 CrO4=7.5*10^-5;//Solubility of CrO4 component in mol
    per litre//
7 Ksp=Ag*CrO4;//value of Ksp//
8 printf('\nValue of Ksp for the reaction=Ksp=%f
    =1.7*10^-12',Ksp);
9 MWAgCl=143.5;//Molecular weight of AgCl//
10 Ksp1=1.1*10^-10;//Ksp value of AgCl//
11 S1=sqrt(Ksp1);//Solubility of AgCl in mol per litre
    //
12 printf('\nSolubility of AgCl=S1=%f=1.05*10^-5mol per
    litre',S1);
13 s1=S1*MWAgCl;//solubility of AgCl in g per litre//
14 printf('\nSolubility of AgCl=s1=%f=1.50*10^-3gram
    per litre',s1);
```

Scilab code Exa 7.26 Solubility product

```
1 MW=372;//molecular weight of Li3Na3(AlF6)2 in grams
    //
2 s=0.74;//solubility of Li3Na3(AlF6)2 in g per litre
    //
3 S=s/MW;//Solubility of Li3Na3(AlF6)2 in mol per
    litre//
4 printf('Solubility of Li3Na3(AlF6)2=S=%fmol per
    litre',S);
5 Li=3*S;//Solubility of Li component in mol per litre
    //
6 Na=3*S;//Solubility of Na component in mol per litre
    //
7 AlF6=2*s;//Solubility of AlF6 component in mol per
    litre//
8 Ksp=(Li^3)*(Na^3)*(AlF6^2);//value of Solubility
    product//
```

```
9 printf('\nValue of Ksp for the reaction=Ksp=%f
    =7.47*10^-19',Ksp);
```

Scilab code Exa 7.27 Concentrations of ions

```
1 Ksp=2.2*10^-8;//Solubility product of PbSO4//
2 Pb=0.01;//concentration of Pb in Pb(NO3)2//
3 SO4=Ksp/Pb;//Concentration of SO4 in PbSO4 solution
    //
4 printf('Let us first calculate the maximum
    concentration of SO4 that can remain in
    equilibrium with PbSO4 if the concentration of Pb
     is 0.01M');
5 printf('\nConcentration of SO4 in PbSO4 solution=Ksp
    =2.2*10^-6M\nThe concentration of SO4 should be
    greater than 2.2*10^-4M in order to precipitate
    Pb from a 0.01M solution as PbSO4');
6 Pb2=Ksp/0.001;
7 printf('\nConcentration of Pb in PbSO4 solution=Pb2
    =2.2*10^-5mol per litre');
8 printf('\nHence out of 0.01moles of Pb in a litre
    only 2.2*10^-5mol per litre remain in solution.
    the precipitation is almost 99.78percent complete
    .');
9 printf('\nTherefore it can be said that Pb is
    quantitatively precipitated in these conditions.'
    );
```

Scilab code Exa 7.28 Concentrations of ions

```
1 Cu=0.1;//concentration of Cu2+ ions in the solution
    //
```

```
2 Mn=0.1;//concentration of Mn2+ ions in the solution
    //
3 H=0.3;//concentration of H+ ions in the solution//
4 KspCuS=1.0*10^-44;//Solubility product of CuS//
5 KspMnS=1.4*10^-15;//Solubility product of MnS//
6 K1=9.1*10^-8;//K1 value of the H2S solution//
7 K2=1.2*10^-15;//K2 value of the H2S solution//
8 K=K1*K2;//K value of H2S//
9 printf('K value of H2S solution=K=1.1*10^-22');
10 S2=K/H^2;//Concentration of S2- in the solution//
11 printf('Concentration of S2 in the solution
    =1.22*10^-22\nThe Iconic product of CuS
    =1.22*10^-22*10^-1 is >> Ksp for CuS and so it
    precipitates.');
12 printf('\nIf MnS were to precipitate the S2 should
    be greater than the equilibrium concentration of
    S2\ni.e Mn*S2 = 1.4*10^-15 so S2eq=1.4*10^-14');
13 printf('\nThe S2 should be greater than 1.4*10^-14
    so that MnS will precipitate.\nLet the S2 desired
     be 1.1*10^-11\nIn order to get this
    concentration of S2 the required H is 10^-6M');
14 printf('\nThe solution should have a PH of greater
    than 6 i.e PH >> 6');
```

Scilab code Exa 7.29 precipitation of cation

```
1 Al=0.01;//concentration of Al3+ ions in the solution
    //
2 Mg=0.01;//concentration of Mg2+ ions in the solution
    //
3 NH4Cl=2;//concentration of NH4Cl in the solution//
4 printf('NH3 + H2O = NH4+ + OH-');
5 KspMgOH2=3.4*10^-11;//Solubility product of Mg(OH)
    2//
6 KspAlOH3=5.0*10^-33;//Solubility product of Al(OH)
```

```
    3//
7 Kb=1.8*10^-5;//Kb value of the NH3//
8 printf('\nNH4+ in solution = NH4+ from added NH4Cl
    that derived from the reaction between NH3 and
    H2O = NH4+ from NH4Cl(since the other quantity is
     too small)');
9 printf('\nNH3 = Original concentration since amount
    dissociated is very low\nwe get OH- = 1.8*10^-5\
    nThe iconic product for Mg(OH)2 is (Mg2+)(OH-)^2
    or (10^-2)(1.8*10^-5)^2 i.e 3.24*10^-12\nIt is
    less than 3.4*10^-11,Ksp,So it is not
    precipitated.');
10 printf('\nHowever,in the case of Al(OH)3 the Iconic
    product=(10^-2)(1.8*10^-5)^3=5.832*10^-17>>The
    Ksp for Al(OH)3 i.e 5.0*10^-33.');
11 printf('\nso Al(OH)3 gets precipitated.');
```

Scilab code Exa 7.30 PH of the solution for precipitation

```
1 Fe=0.01;//concentration of Fe3+ ions in the solution
    //
2 Ksp=3.8*10^-38;//Solubility product of Fe(OH)3//
3 OH=(Ksp/Fe)^0.333;//Concentration of OH- ions in the
     solution//
4 printf('Concentration of OH- ions in the solution=OH
    =%f=1.561*10^-12',OH);
5 printf('\nAt this PH,Fe(OH)3 starts precipitating
    and precipitation is complete (Fe3+)=10^-6M\n
    (10^-6)(OH-)^3 = 3.8*10^-38 ');
6 printf('\nupon solving this we get (OH-)
    =3.362*10^-11\nPOH=10.48 or PH=3.52');
7 printf('\nAt this PH the precipitation of Fe(OH)3 is
     almost complete.');
```

Scilab code Exa 7.31 Solubility of CaF2

```
1 C=0.01;//concentration of Ca(NO3)2 solution//
2 Ksp=3.2*10^-11;//Solubility product of Fe(OH)3//
3 printf('CaF2 = Ca2+ + 2F-\n(Ca2+)(F-)^2 = 4*S^3 =
    3.2*10^-11.');
4 printf('\nLet S1 be the solubility in 0.01M Ca(NO3)
    2\nCa(NO3)2 can be assumed to dissociate
    completely so that (Ca2+) from Ca(NO3)2 is 0.01M'
    );
5 S=(Ksp/4)^0.33;//solubility in mol per litre//
6 printf('\nSolubility of CaF2 solution=S=%f
    =2.18*10^-4mol per litre',S);
7 printf('\nThe solubility product relationship should
     be true,irrespective of the source Ca2+\
    nCompared to the concentration of Ca2+ ions
    obtained from Ca(NO3)2,that of Ca2+ ions from
    CaF2 is negligible');
8 S1=sqrt(Ksp/0.04);//solubility in 0.01M ca(NO3)2//
9 printf('\nBut the F- ions are obtained only from
    CaF2 and so (F-)=2*S1\nKsp = 3.2*10^-11=(S1+0.01)
    *(2*S1)^2=(0.01)*(2*S1)^2 since S1 is negligible
    compared to 0.01');
10 printf('\nSolubility in 0.01M Ca(NO3)2 solution=S1=
    %f=2.83*10^-5',S1);
11 printf('\nThus the value of S1 can be seen to be
    less than that of S');
```

Scilab code Exa 7.32 dG dH dS of the reaction

```
1 T=298;//temperature in kelvin//
2 E=0.22;//emf of the cell in volts//
```

```
dE=-0.00065;//Temperature coefficient of the emf in
    volt per degree//
c=4.184;//1 cal =4.184 joules//
n=1;
F=96500;//1Farad value//
printf('The positive electrode is the cathode and
    the negative electrode is the anode in a galvanic
     cell\nAnode reaction 1/2H2 = H+ + e-\nCathode
    reaction AgCl + e- = Ag+ + Cl-\nCell reaction 1/2
    H2 + AgCl = Ag+ + H+ + Cl-');
dG=-n*F*E/c;//free energy change in the cell in cal
    per mol//
printf('\nFree energy change in the cell=dG=%fcal
    per mol',dG);
dH=dG+(n*F*T*dE/c);//Enthalpy change in the cell//
printf('\nEnthalpy change in the cell=dH=%fcal per
    mol',dH);
dS=(dH-dG)/T;//Entropy change in the cell in cal per
     deg//
printf('\nEntropy change in the cell=dS=%fcal per
    deg',dS);
```

Chapter 8

Chemical Kinetics and Catalysis

Scilab code Exa 8.3 First order rate constant and half life

```
1 k=1.37*10^-4;//rate constant in per sec//
2 thalf=5057;//half time of the reaction in sec//
3 printf('If out of each mole of N2O5,x mole of it
    decomposes at any instant\nThe total pressure in
    the system is equal to that due to (1-x)moles of
    undecomposed N2O5,\nx moles of N2O4 and x/2moles
    of O2 i.e due to 1+(x/2)moles.');
4 printf('\nThe increase in pressure is thus due to x
    /2moles\nSo the amount of N2O5 that has
    decomposed at any instant i.e x is proportional
    to twice the observed increase in pressure');
5 printf('\nThese can be fitted into the kinetic
    equation for a first order reaction\nk=(2.303/t)*
    log10(a/(a-x))\nand the value of k can be
    obtained.The average value of k is 1.37*10^-4per
    sec');
6 printf('\nk=0.693/t0.5 that will result in t0.5=5057
    seconds\nThis can also be obtained as the value
    corresponding to (a-x)=154.1mm,from a graph of t
```

```
vs (a-x).');
```

Scilab code Exa 8.4 First order rate constant

```
1 Vinfinite=58.3;//volume of nitrogen evolved at
    infinite time//
2 V0=19.3;//volume of nitrogen evolved at initial time
    //
3 printf('Let V0,Vt,Vinfinite be the volumes of N2
    evolved at the beginning,at time t and at
    infinite time(no more collection of N2 is
    observed)respectively,');
4 printf('\n(Vinfinite-V0)is a measure of the total
    amount of material that can decompose,\ni.e the
    initial concentration a.\n(Vinfinite-Vt) is a
    measure of the amount of material that remains
    unreacted at time t,i.e (a-x),\nbecause this
    volume corresponds to the amount of material that
     can still decompose between time t and infinite
    time.');
5 printf('\nk=(2.303/t)*(log10((Vinfinte-V0)/(
    Vinfinite-Vt))).');
6 printf('\nThe average value of k can be found to be
    6.54*10^-2per min or 1.09*10^-3per sec');
```

Scilab code Exa 8.5 Minimum initial activity

```
1 t=12.8;//half life of the particle in hours//
2 k=0.693/(t*60);//value of k for the experiment in
    per min//
3 printf('Value of k for the experiment=k=%fper min',k
    );
```

```
4 printf('\n-dN/dt=rate=100*k*N=(0.693/12.8*60)*N\nN,
    the number of copper atoms required to produce
    100Beta particles per minute\n we get N
    =(100*12.8*60)/0.693=1.108*10^5');
5 w=63.5;//atomic weight of Cu in grams//
6 AN=6.023*10^23;
7 N=1.108*10^5;
8 W=(N*w)/AN;//weight of Cu in grams//
9 printf('\nWeight of Cu=W=%f=1.17*10^-17grams',W);
10 printf('\nSince the maximum activity is 100Beta
    particles per minute,N=(a-x) at the end of six
    hours,i.e t=6 and N=1.108*19^5atoms');
11 printf('\nAt zero time N0=a\n a-x=a*exp(-k*t)\nUpon
    solving the above equation we get N0=a=1.533*10^5
    atoms\nWeight of Cu to start with=1.66*10^-17
    grams.');
12 printf('\nInitial activity=138.30000 disintegrations
    per minute');
```

Scilab code Exa 8.7 Specific reaction rate

```
1 printf('The kinetic equation for a second order
    reaction involving unequal concentrations of the
    reactants is\nk2=(2.303/(t*(a-b)))*log10((b*(a-x)
    )/(a*(b-x)))');
2 k=2.312*10^-4;
3 p=4.94*10^-3;//value of (a-b)//
4 k2=(k*2.303)/p;//second order reaction rate//
5 printf('\nSecond order reaction rate=k2=%flitre per
    mol per second',k2);
```

Scilab code Exa 8.8 Order of the reaction

```
t1half=37.00;//half time for the first order
   reaction//
t2half=19.2;//half time for the second order
   reaction//
t3half=9.45;//half time for the third order reaction
   //
printf('to know the order of the equation we can use
    2^(n-1)=t1half/t2half');
printf('\nby solving for first and second order n
   =1.95\nby solving for second and third order n
   =2.02');
printf('\nby solving for first and third order n
   =1.98\nSo the order of the reaction=n=2');
```

Scilab code Exa 8.10 Pseudo first order Rate constant

```
k=8.676*10^-3;//average value of k in per min//
printf('Average value of k=8.676*10^-3per min');
r0=22.4;
rt=0;
rinfinite=-11.1;
t=(2.303/k)*log10((r0-rinfinite)/(rt-rinfinite));
printf('\nThe time at which the mixture is optically
    inactive=t=%fmin',t);//here in textbook the
   answer is given wrong,but by solving we get the
   same result as executed//
```

Scilab code Exa 8.13 Order of the reaction

```
k=1;
a=10;
thalf=10^-1.88;//half time of the reaction//
```

```
4 n=1-(log10(thalf/k)/log10(a));//order of the
    reaction//
5 printf('order of the reaction after solving is n=%f'
    ,n);
6 printf('\nHence the order of the reaction=n=3');
```

Scilab code Exa 8.14 Half life of the reaction

```
1 thalf1=49;//half life for 0.02M compound//
2 thalf2=100;//half life for 0.04M compound//
3 M1=0.02;//initial concentration of the compound//
4 M2=0.01;//Final concentration of the compound//
5 printf('Since thalf is directly proportional to
    concentration(doubling the concentration
    increases thalf by a factor 2),\nthe reaction is
    Zero order.\nThe half time corresponding to a
    concentration of 0.01M will be 24.5mins');
```

Scilab code Exa 8.18 Energy of activation

```
1 R=1.987;//universal gas constant//
2 T1=293;//initial temperature in kelvin//
3 T2=303;//Final temperature in kelvin//
4 K1=6.68*10^-3;//rate constant corresponding to T1 in
    per min//
5 K2=1.31*10^-2;//rate constant corresponding to T2 in
    per min//
6 E=(2.303*R*T1*T2*log10(K2/K1))/(T2-T1);//energy of
    activation in Kcal per mol//
7 printf('Energy of activation=E=%fcal per mol=11.88
    Kcal per mol',E);
```

Scilab code Exa 8.19 Ratio of reaction rates

```
1 R=1.987;//universal gas constant//
2 T1=350;//initial temperature in kelvin//
3 T2=360;//Final temperature in kelvin//
4 E=40000;//energy of activation in cal per mol//
5 K=10^(E*((T2-T1)/(T1*T2))/(2.303*R));//ratio of v2/
    v1//
6 printf('The ratio of V2 and V1 is K=V2/V1=%f',K);
```

Scilab code Exa 8.20 Activation energy

```
1 R=1.987;//universal gas constant//
2 T1=313;//initial temperature in kelvin//
3 T2=333;//Final temperature in kelvin//
4 t1=15;//time for 20% reaction at 313K in mins//
5 t2=3;//time for 20%reaction at 333K in mins//
6 K=t1/t2;//ratio of K2/K1//
7 E=(2.303*R*T1*T2*log10(K))/(1000*(T2-T1));//energy
    of activation in Kcal per mol//
8 printf('Energy of activation=E=%fKcal per mol',E);
```

Scilab code Exa 8.21 Arrhenius constant

```
1 R=1.987;//universal gas constant//
2 printf('From the graph slope=(-0.92/0.30)=(-E
    /(2.303*R))\nGraphical evaluation of A requires
    the determination of the intercept on the y axis
    corresponding to 1/T=0\nOne can also calculate A
    from k=A*exp(-E/(R*T))');
```

```
3 E=(0.92*R*2.303)/(0.30*10^3);
4 printf('\nEnergy of activation=E=%f=14.04Kcal per
    mol',E);
5 k=2.31*10^-2;
6 T=273;//temperature in kelvin//
7 printf('\nwe can find the value of A using log10(k)=
    log10(A)-(E/(2.303*R*T))\nUpon solving we get A
    =4.015*10^9litre per mol per second');
```

Scilab code Exa 8.22 Rate constant

```
1 R=1.987;//universal gas constant//
2 T=556;//temperature in kelvin//
3 E=44;//Energy in Kcal//
4 dS=-10;//entropy change in cal per deg//
5 k=(exp(2)*exp(dS/R)*exp(-E/(R*T))*10^13.07);//rate
    constant for the reaction//
6 printf('Rate constant for the reaction=k=3.47*10^-7
    litre per mol per sec');
```

Scilab code Exa 8.23 Standard Entropy change

```
1 R=1.987;//universal gas constant//
2 T=473;//temperature in kelvin//
3 A=2.75*10^15;//frequency factor in per sec//
4 K=1.38*10^-16;//boltzmans constant//
5 h=6.625*10^-27;//planks constant//
6 dn=0;
7 dS=4.57*(log10(A)-log10(exp(1))-log10(9.85*10^12));
    //entropy change in cal per deg//
8 printf('The entropy of activation=dS=%f=9.19eu',dS);
9 printf('\nSince A is independent of concentration
    units dS does not sepend on the concentration
```

```
    units used\nand hence the standard state.\
    nHowever if the time were expressed in different
    units A will assume a different value\nand
    consequently the value of dS will be different\
    nIf time were expressed in minutes A
    =2.75*10^15*60 per min\ndS=9.19+4.57*log10(60)
    =17.32eu\nfor bimolecular reaction e^2=7.4*10^10
    \nso dS will result in dS=-10.1eu or mol per
    litre.');
10 printf('\nIf the concentration were expressed in mol
     per millilitre A would be 7.4*10^13 \nso dS will
     result in dS=-10.1+13.6=3.5eu or mol per
    millilitre\nIf the concentration were expressed
    in molecules per millilitre the value of A will
    be multiplied by 6.023*10^23 \nso dS would result
     in as dS=-10.1-94.9=-105eu or -105molecules per
    millilitre');
```

Chapter 9

PHOTOCHEMISTRY

Scilab code Exa 9.1 Optical path of the cell

```
1 printf('Let M be the Molecular weight of the dye.
    Original concentration is 30.1/M mol litre^-1');
2 I0=100;
3 I=50;
4 b=1;
5 A=log10(I0/I);
6 printf('\nFrom Beers law=A=%f',A);
7 x=A/30.1;
8 printf('\na/M=%f',x);
9 c=15.05;
10 I=70.7;
11 printf('\nPercentage of light transmitted=I=%f',I);
12 AI=100-I;
13 printf('\nPercentage of light absorbed=AI=%f',AI);
14 c=60.2;
15 I=25;
16 printf('\nPercentage of light transmitted=I=%f',I);
17 AI=100-I;
18 printf('\nPercentage of light absorbed=AI=%f',AI);
19 printf('\nIt must be noted that it is absorbance A
    that is linearly related to concentration and not
```

```
    percentage light transmitted or absorbed');
b=2;
c=30.1;
I=25;
printf('\nPercentage of light transmitted=I=%f',I);
b=4.32;
printf('\nb=%fcm',b);
```

Scilab code Exa 9.2 Rate of formation

```
c=3*10^10;//velocity of light in cm//
h=6.625*10^-27;//plank's constant//
L=6.02*10^23;//Avagadro number//
l=3020*10^-8;//wavelength of light radiation in cm//
E=(L*h*c)/l;//value of one einstein in ergs//
printf('Value of one einstein=E=%f=3.96*10^12ergs',E
   );
LA=15000;//light absorbed in ergs per second//
NE=LA/E;//number of einsteins absorbed per second//
printf('\nNumber of Einsteins absorbed per second=NE
   =3.788*10^-9');
QY=0.54;//Quantum yield for CO formation//
N=QY*NE;//number of moles of CO formed per sec//
printf('\nNumber of moles of Co formed per sec=N
   =2.046*10^-9');
R=2.046*10^-9;//Rate of formation of CO in moles per
    sec//
printf('\nRate of formation of CO=R=2.046*10^-9
   moles per sec');
```