Scilab Textbook Companion for
Physical Chemistry for the Chemical and Biological Sciences
by Raymond Chang[1]

Created by
Anjali Kotecha
master in science
Others
pandit ravisankar university raipur
College Teacher
None
Cross-Checked by
None

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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.

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Chapter 2

The Gas Laws

Scilab code Exa 2.1 `Calucate the number of oxygen molecules`

```

//Calculate the number of oxygen molecules
//Example 2.1

clc;

clear;

r=0.0050;.......//radius of alveoli in cm

P=1;........//Pressure in atm

R=0.08206;.......//Gas Constant in L atm K^-1 mol^-1

T=310;.......//Temperature in Kelvin

mp=14;........//Mole Percent of Oxygen

V=(4/3)*%pi*r^3*10^-3;........//Volume of one
    alveolus in Litres

```

```
n=(P*V)/(R*T);..........//Number of moles of air in one alveolus in mol

Na=6.022*10^23;.....//Avagadro's Number

N=n*(mp/100)*Na;.......//Number of Oxygen Molecules

printf("The number of oxygen molecules = %.1f*10^12 Oxygen molecules",N*10^-12);
```

Scilab code Exa 2.2 `Calculate the mass of Oxygen`

```
//Calculate the mass of Oxygen

//Example 2.2

clc;

clear;

PT=758;     //Total partial pressure in torr

PH2O=19.8;    //Partial pressure of water in torr

PO2=(PT-PH2O)*0.00131579;     //Partial pressure of oxygen in torr

V=0.186;    //Volume of oxygen in Litre

M=32;    //Molar mass of oxygen in g/ mol

R=0.08206;   //Gas constant in L atm K^-1 mol^-1

```

```
T=295;    //Tempreture in kelvin

m=(PO2*V*M)/(R*T); //Mass of the Oxygen molecule in g

printf(”Mass of Oxygen molecule = %.3f g”,m);
```

Scilab code Exa 2.3 `Calculate the pressure of gas if Nitrogen behaves as a Van der`

```
//Calculate the pressure of  gas if Nitrogen behaves as a Van der Waals and ideal gas

// Example 2.3

clc;

clear;

n=2000;  //Number of Nitrogen molecule in mol

R=0.08206;  //Gas constant in L atm K^-1 mol^-1

T=898;  //Tempreture in kelvin

V=800;   //Volume of vessel in L

b=0.0386;  //Van der walls constant in L /mol

a=1.35;  //Proportionality constant in L^2/mol^2

P1=((n*R*T)/(V-(n*b)))-((a*n^2)/(V^2)); //Pressure of gas in atm

```

```
printf("(a) Pressure of gas when Nitrogen behaves as Van Der Valls Gas = %.0f atm",P1);

P2=(n*R*T)/V; //Pressure of gas if Nitrogen behaves as an ideal gas

printf("\n(b)Pressure of gas if Nitrogen behaves as an ideal gas = %.0f atm",P2);
```

Scilab code Exa 2.4 `Calculate the molar volume of Methane`

```
//Calculate the molar volume of Methane

//Example 2.4

clc;

clear;

B=-0.042;  //Second virial coefficient of Methane in L mol^-1

P=100;    //Pressure in atm

R=0.08206;  //Gas constant in L atm K^-1 mol^-1

T=300;  //Temperature in kelvin

Z=1+((B*P)/(R*T));  //Compressibility Factor

Vbar=(Z*R*T)/P;//Volume of Methane per mol in L

printf("Observed Molar Volume of Methane = %.2f L
```

```
    mol^-1", Vbar);

V1bar=(R*T)/P; //Molar volume of Methane through
    Ideal Gas Equation in L

printf("\nMolar volume of Methane through Ideal Gas
    Equation = %.2f L mol^-1", V1bar);
```

Chapter 3

Kinetic Theory of Gases

Scilab code Exa 3.1 `Calculate the Most probable speed Mean speed and Root mean squ`

```
//Calculate the Most probable speed ,Mean speed and Root mean square speed for Oxygen molecule

//Example 3.1

clc;

clear;

R=8.314;    //Gas constant in J K^-1 mol^-1

T=300;  //Temperature in kelvin

mew=0.03200;  //Molar mass of Oxygen kg mol^-1

Cmp=sqrt((2*R*T)/(mew))//Most probable speed in m s^-1

printf("most probable speed = %.0f m s^-1",Cmp);

Cbar=sqrt((8*R*T)/(%pi*mew)); //Mean speed in m s^-1
```

```

printf("\nMean speed = %.0f m s^-1",Cbar);

Crms=sqrt((3*R*T)/(mew)); //Root mean square speed in m s^-1

printf("\nroot mean square speed = %.0f m s^-1",Crms);
```

Scilab code Exa 3.2 `Calculate the Collision frequency Binary Collision Number and`

```

//Calculate the Collision frequency Binary Collision Number and Mean free path of Nitrogen

//Example 3.2

clc;

clear;

R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;  //Temperature in Kelvin

mew=0.02800;  //Molar mass of Nitrogen in Kg mol^-1

Cbar=sqrt((8*R*T)/(%pi*mew))*100; //Average speed of Nitrogen in cm/s

Conc=2.5*10^19; //Concentration of dry air in cm^-3

Cd=3.75*10^-8;  //Collision diameter in cm
```

```

Z1=sqrt(2)*%pi*(Cd)^2*Cbar*Conc;....//Collision frequency in collisions s^-1

printf("Collision frequency of Nitrogen = %.1f*10^9 collisions s^-1",Z1*10^-9);//(The answers vary due to round off error)

Z11=(Z1/2)*Conc;....//Binary Collision number in cm^-3 s^-1

printf("\nBinary collision number = %.1f*10^28 collisions cm^-3 s^-1",Z11*10^-28);

lambda=Cbar/Z1; //Mean free path of Nitrogen in A/collision

printf("\nMean free path of Nitrogen = %.0f* A/collision",lambda*10^8);
```

Scilab code Exa 3.3 `Calculate the Viscosity of Oxygen gas`

```
//Calculate the Viscosity of Oxygen gas

//Example3.3

clc;

clear;

R=8.314;   //Gas constant in J K^-1 mol^-1

T=288;   //Temperature in K
```

```
mew=0.03200;  //Molar mass of Oxygen in kg mol^-1

Cbar=sqrt((8*R*T)/(%pi*mew)); //Mean speed of Oxygen in m s^-1

d=3.61*10^-10;  //Collision diameter of Oxygen in m

M=32*1.661*10^-27;  //Mass of Oxygen in kg

eta=(M*Cbar)/((3*d^2*%pi)*sqrt(2));  //Viscosity of Oxygen in kg m^-1 s^-1

printf("Viscosity of Oxygen gas = %.2f*10^-5 kg m^-1 s^-1",eta*10^5);
```

Scilab code Exa 3.4 `Calculate the mass of Carbon di Oxide in gramm that collides e`

```
//Calculate the mass of Carbon di Oxide in gramm that collides every second with leaf

//Example 3.4

clc;

clear;

P=(0.033*101325*1)/(100*1);  //Partial pressure of the gas in Pa

M=44.01*1.661*10^-27;  //Molecular mass of CO2 in kg

R=8.314;  //Gas constant in J K^-1 mol^-1
```

```

NA=6.023*10^23; // Avagadro number mol^-1

Kb=R/NA;  //Boltzman's constant in J K^-1

T=298;  //Tepmerature in K

ZA=P/(2*%pi*M*Kb*T)^0.5;

A=0.020;  //Area of leaf in m^2

Noc=ZA*A; //Number of CO2 molecule colliding with
   the leaf in s^-1

Moc=Noc*7.31*10^-23;  //Mass of CO2 that colliding
   with leaf in g s^-1

printf("Mass of Carbon di Oxide that collide = %.1f
   g s^-1",Moc);
```

Chapter 4

The First Law of Thermodynamics

Scilab code Exa 4.1.a `Calculate the value of work done if the expansion is carried`

```


//Calculate the value of work done if the expansion is carried out against a vacuum ,against a constant external pressure of 1.00 atm and reversibly

//Example 4.1

clc;

clear;

n=0.850;   //Number of mole of gas in mol

R1=0.08206; //Gas constant in L atm K^-1 mol^-1

T=300;   //Temperature in K

```

```
P1=15.0;  //Initial pressure in atm

P2=1.00;  //Final pressure in atm

Pex=0;  //Pressure in vaccum

V1=(n*R1*T)/P1; //Initial volume in Litres

V2=(n*R1*T)/P2;  //Final volume in Litres

w1=-Pex*(V2-V1)*101.3;  //Work done against vaccum in J

printf("(a)Work done if the expansion is carried out against a vaccum = %.0f J",w1);

w2=-P2*(V2-V1)*101.3;  //Work done against a constant external pressure in J

printf("\n(b)Value of work done if the expansion is carried out against a constant external pressure = %.2f*10^3 J",w2*10^-3);

R2=8.314;  //Gas constant in J K^-1 mol^-1

w3=(-n*R2*T)*log((P1/P2));  //Work done for an isothermal,reversible process in J

printf("\n(c)Work done if the expansion is carried out for an isothermal,reversible process = %.2f*10^3 J",w3*10^-3);
```

Scilab code Exa 4.1 `Calculate the value of work done if the expansion is carried o`

```
//Calculate the value of work done if the expansion is carried out against a vacuum ,against a constant external pressure of 1.00 atm and reversibly

//Example 4.1

clc;

clear;

n=0.850;  //Number of mole of gas in mol

R1=0.08206; //Gas constant in L atm K^-1 mol^-1

T=300;  //Temperature in K

P1=15.0;  //Initial pressure in atm

P2=1.00;  //Final pressure in atm

Pex=0;  //Pressure in vaccum

V1=(n*R1*T)/P1; //Initial volume

V2=(n*R1*T)/P2;  //Final volume

w1=-Pex*(V2-V1)*101.3;  //Work done against vaccum in J

printf("(a)Work done if the expansion is carried out against a vaccum = %.0f J",w1);

w2=-P2*(V2-V1)*101.3;  //Work done against a constant external pressure in J

printf("\n(b)Value of work done if the expansion is carried out against a constant external pressure
```

```
 = %.2f*10^3 J",w2*10^-3);

R2=8.314;   //Gas constant in J K^-1 mol^-1

w3=(-n*R2*T)*log((P1/P2));   //Work done for an isothermal,reversible process in J

printf("\n(c)Work done if the expansion is carried out for an isothermal,reversible process = %.2f*10^3 J",w3*10^-3);
```

Scilab code Exa 4.2 How high the person can climb on this energy intake

```
//How high the person can climb on this energy intake

//Example4.2

clc;

clear;

M=73;   //Weight of the person in kg

m=500;   //Mass of milk that person drink in g

Cv=720;   //Caloric value of milk in cal g^-1

Mw=17;   //Percant of milk that converted in mechanical work

W=(Mw*m*Cv*4.184)/100;   //Energy intake for mechanical work in J
```

```

g=9.81;  //Acceleration due to gravity in m s^-2

h=W/(M*g); //Person climb by this height in m

printf("The person climbs to a height = %.1f*10^2 m",h*10^-2);
```

Scilab code Exa 4.3 `Calculate the value of change in Internal energy and change in`

```

//Calculate the value of change in Internal energy and change in Enthalpy for the combution of Benzoic acid

//Example 4.3

clc;

clear;

C=5267.8;  //Effective heat capcity of bomb calorimeter plus water im J K^-1

T1=293.32;  //Initial temperature in K

T2=295.37;  //Final temperature in K

delT=T2-T1;  //Change in teperature in K

M=122.12;  //Molar mass of Benzoic acid in g mol^-1

m=0.4089;  //Mass of sample of Benzoic acid in g
```

```

delU=-(C*delT*M)/(m*1000);  //Change in Enternal enegy in kJ mol^-1

printf("Change in Internal energy = %.0f kJ mol^-1",delU);//(The answer vary due to round off error)

R=8.314;  //Gas constant in J K^-1 mol^-1

T=T1; //Temperature in K

n1=7.5;  //Number of moles of gas for reactants

n2=7;  //Number of mole of gas for product

deln=n2-n1;  //Change of moles gas for reaction

delH=delU+((R*T*deln)/1000); //Change in Enthalpy in kJ mol^-1

printf("\nChange in Enthalpy = %.0f kJ mol^-1",delH);
```

Scilab code Exa 4.4 `Compare the difference between change in Enthalpy and change i`

```
//Compare the difference between change in Enthalpy and change in Enternal energy for 1 mol of ice melt  in to 1 mol of water at 273 K and one mole water change in to one mole steam at 373 K

//Example4.4

clc;
```

```

clear;

Vbars=0.0196;  //Molar volume of ice in L mol^-1

Vbarl=0.0180;  //Molar volume of water in L mol^-1

P=1;  //Pressure in atm

delV1=Vbarl-Vbars;  //Change in molar volume when water change in to steam in L mol^-1)

E1=P*100*delV1;  //Differerce between change in Enthalpy and change in Enternal energy when ice melt in to water in J mol^-1 delH-delU

printf("(a)Difference between change in Enthalpy and change in Enternal energy for 1 mol of ice melt in to 1 mol of water at 273 K = %.2f J mol^-1",E1);

Vbarg=30.61;  //Molar volume of steam in L mol^-1

delV2=Vbarg-Vbarl;  //Change in molar volume when water change in to steam in L mol^-1)

E2=P*101.33*delV2;  //Differerce between change in Enthalpy and change in Enternal energy when water change in to steam delH-delU in J mol^-1

printf("\n (b)Difference between change in Enthalpy and change in Enternal energy for one mole water change in to one mole steam at 373 K  = %.0f J mol^-1",E2);
```

Scilab code Exa 4.5 Calculate the change in Enternal energy and change in Enthalpy

```
//Calculate the change in Enternal energy and change in Enthalpy for heating of Xenon

//Example4.5

clc;

clear;

T1=300;  //Initial temperature in K

T2=400;  //Final temperature in K

m=55.40;  //Mass of Xenon in g

M=131.29;  //Molecular mass of Xenon

n=m/M;  //Number of mole of Xenon in mol

R=8.314;  //Gas constant in J K^-1 mol^-1

Cbarv=(3/2)*R;  //Molar constant volume in J K^-1 mol^-1

delT=T2-T1;  //Thange in temperature in K

delU=n*delT*Cbarv;  //Change in Enternal energy in J

```

```
printf(”Change in Enternal energy = %.0f J”,delU);

Cbarp=(5/2)*R;  //Molar constant pressure in J K^−1
   mlo^−1

delH=n*Cbarp*delT;  //Change in Enthalpy in J

printf(”\nChange in Enthalpy = %.0f J”,delH);
```

Scilab code Exa 4.6 Calculate the Enthalpy Change for heating of Oxygen molecule

```
//Calculate the Enthalpy Change for heating of 1.46
   moles of Oxygen

//Example 4.6

clc;

clear;


n=1.46;   //Number of moles of Oxygen

function x=Cp(T) ,x=(25.7+0.0130*T), endfunction
          //Molar Heat Capacity of Oxygen at
   Constant Pressure in J K^−1 mol^−1

function y=f(T),y=n*Cp(T),endfunction

delH=intg(298,367,f);     //Enthalpy Change in J

printf(”Enthalpy Change = %.2f*10^3 J”,delH*10^-3)
```

Scilab code Exa 4.7 Calculate the work done if the expansion is carried out Adiaba

```
//Calculate the  work done if the expansion is carried out Adiabatically and Reversibly

//Example 4.7

clc;

clear;

n=0.850;  //Number of moles of momnoatomic ideal gas in mol

R=0.08206;  //Gas constant in L atm K^-1

T1=300;  //Initial temperature in K

P1=15;  //Initial pressure in atm

V1=(n*R*T1)/P1;  //Initial volume in L

P2=1;  //Final pressure in atm

gama=5/3; //Constant for Adiabatic Expansion

V2=V1*(P1/P2)^(1/gama);  //Final volume in L

T2=(P2*V2)/(n*R);  //Final temperature in K

Cbarv=12.47;  //Molar consant volume heat capacity in J K^-1 mol^-1
```

```

delU=n*Cbarv*(T2-T1);  //Change in Enternal energy
   in J

w=delU;  //Change in Enternal energy converted in to
    amount of work done in expansion is carried out
   Adiabatically and Reversibly in J

printf("Work done = %.1f*10^3 J",w*10^-3);
```

Scilab code Exa 4.8 `Calculate the standard molar Enthalpy of formatyion of Acetyle`

```
//Calculate the standard molar Enthalpy of
   formatyion of Acetylene (C2H2) from its element

//Example 4.8

clc;

clear;

delH1deg=-393.5;  //Enthalpy change for the reaction
    C(graphite)+O2(g) givs CO2(g) in kJ mol^-1

delH2deg=-285.8;  //Enthalpy change for the reaction
    H2(g)+1/2O2(g) givs H2O(l) in kJ mol^-1

delH3deg=-2598.8;  //Enthalpy change for the
   reaction 2C2H2(g)+5O2(g)givs 4CO2(g)+2H2O(l)in kJ
    mol^-1

delH4deg=-delH3deg;  //Enthalpy change for the
   reaction 4CO2(g)+2H2O(l)givs 2C2H2(g)+5O2(g)in kJ
```

```
    mol^-1

delHdeg=(4*delH1deg+2*delH2deg+delH4deg)/2;  //Molar
    Enthalpy for formation of acetylene in kJ mol^-1

printf("Molar Enthalpy = %.1f kJ mol^-1 ",delHdeg);
```

Scilab code Exa 4.9 Calulate the standard Enthalpy of the reaction

```
//Calulate the standard Enthalpy of the reaction
   C6H12O6(s)+6O2(g)givs 6CO2(g)+6H2O(l)at 298 K

//Examlpe 4.9

clc;

clear;

delfHbar1=-393.5;  //standard Molar Enthalpy of
   formation at 298 K and 1 Bar for CO2 in kJ mol^-1

delfHbar2=-285.8;  //standard Molar Enthalpy of
   formation at 298 K and 1 Bar for H2O in kJ mol^-1

delfHbar3=-1274.5;  //standard Molar Enthalpy of
   formation at 298 K and 1 Bar for C6H12O6 in kJ
   mol^-1

delfHbar4=0;  //standard Molar Enthalpy of formation
    at 298 K and 1 Bar for O2 in kJ mol^-1

delfHbar=(6*delfHbar1+6*delfHbar2)-(delfHbar3+6*
   delfHbar4);  //standard Enthalpy of the reaction
```

```
in kJ mol^-1

printf("Standard Enthalpy of the reaction = %.1f kJ mol^-1",delfHbar);
```

Scilab code Exa 4.10 `Calculate the standard Enthalpy for the reaction three Oxygen`

```
//Calculate the standard Enthalpy  for the reaction three Oxygen molecule givs two Ozone molecule

//Example 4.10

clc;

clear;

delrH298deg=285.4;  //standard enthalpy at 298 k in kJ mol^-1

Cp1=29.4;  //molar heat capacity for O2 at constant pressur in J K^-1

Cp2=38.2;  //molar heat capacity for O3 at constant pressur in J K^-1

delCp=2*Cp2-3*Cp1;  //change in molar heat capacity for reaction in J K^-1

T2=380;  //final temperature in K

T1=298;  //initial temperature in K

delT=T2-T1;  //change in temperature in K
```

```

delrH380deg=((delCp*delT)/1000)+delrH298deg;  //standard Enthalpy for the reaction at 380 K in kJ mol^-1

printf(”Standard Enthalpy = %.1f kJ mol^-1”,delrH380deg);
```

Scilab code Exa 4.11 `Estimate the Enthaply of Combustion for Methane`

```
// Estimate the Enthaply of Combustion for Methane

//Exaample 4.11

clc;

clear;

H1=414; //Bond Enthalpy for a C–H bond in kJ mol^-1

H2=498.8; //Bond Enthalpy for a O–O bond in kJ mol^-1

H3=799;  //Bond Enthalpy for a C=O bond kJ mol^-1

H4=460;  //Bond Enthalpy for a O–H bond kJ mol^-1

delHr=((4*H1)+(2*H2))-((2*H3)+(4*H4)); //Enthalpy of the reaction kJ mol^-1

printf(”Enthalpy Change of combustion of methane = %.1f kJ mol^-1”,delHr);

```

```
H5=-393.5;  //Enthalpy of formation of CO2 kJ mol^-1

H6=-241.8;  //Enthalpy of formation of H2O kJ mol^-1

H7=-74.85;  //Enthalpy of formation of CH4 kJ mol^-1

delHf=(H5+(2*H6))-H7; //Enthalpy of formation kJ mol^-1

printf("\nEnthalpy Change of combustion of methane from enthalpy of formation = %.1f kJ mol^-1",delHf);
```

Chapter 5

The Second Law of Thermodynamics

Scilab code Exa 5.1 `Calculate the Entropy change when Ideal gas are expand to Isot`

```
//Calculate the Entropy change when Ideal gas are expand to Isothermaly ,Estimate the probability that the gas will contract spontaneously from the final volume to initial volume

//Example 5.1

clc;

clear;

n=2;  //Number of moles of gas in mol

R=8.314;  //Gas consant in J K^-1 mol^-1

V2=2.4;  //final volume of the gas in L

V1=1.5;  //initial volume of the gas in L

```

```
delS=n*R*log(V2/V1);  //Entropy change in J K^-1

printf("Entropy change = %.1f J K^-1",delS);

Kb=1.381*10^-23;  //Boltzman's constant in J K^-1

r=exp(-delS/Kb);  //probability for spontaneous
   contraction=W1/W2 (Probability for spontaneous
   contraction is zero  butit must be with the aid
   of external force)

printf("\nProbability for spontaneous contraction =
   %.0f",r);
```

Scilab code Exa 5.2 `Calulate the Efficiency of the power plant`

```
//Calulate the Efficiency of the power plant

//Example 5.2

clc;

clear;

T2=833;  //final temperature in K

T1=311;  //initial temperature in K

e=((T2-T1)*100)/T2;  //Efficiency of the power plant
    in percent

printf("Efficiency of the power plant = %.0f percent
   ",e);
```

Scilab code Exa 5.3 How much work must be done by a heat pump when the outdoor tem

```
//How much work must be done by a heat pump when the outdoor temperature is 5 dgree and minus 10 degree

//Example 5.3

clc;

clear;

q2=5000;  //Amount of heat deliver by a pump in J

T2=295;  //Temperature of house in K

T1=278;  //Outdoor teperature in K

q1=abs(q2)*(T1/T2);  //Amount of heat in J

w1=abs(q2)-q1;  //Amount of work done by a heat pump when the outdoor temperature is 5 dgree in J

printf("(a)Amount of work done when the outdoor temperature is 5 dgree = %.0f J",w1);

T3=263;  //Outdoor teperature in K

q1=abs(q2)*(T3/T2);  //Amount of heat in J

w2=abs(q2)-q1;  //Amount of work done by a heat pump in J
```

```

printf("\n(b)Amount of work done when the outdoor temperature is minus 10 degree = %.0f J",w2);
```

Scilab code Exa 5.4 `Calculate the Entropy change for the system for the surroundin`

```
//Calculate the Entropy change for the system ,for the surrounding and for the universe expands isothermally against a constant pressure

//Example 5.4

clc;

clear;

n=0.50;  //Number of moles of Ideal gas in mol

R=8.314;  //Gas constant in J K^-1 mol^-1

V2=5.0;  //Final volume of the gas in L

V1=1.0;  //Initial volume of the gas in L

delSsys=(n*R)*log(V2/V1);  //Entropy change for the system in J K^-1

printf("Entropy change for the system = %.1f J K^-1",delSsys);

P=2;  //Pressure of the gas in atm

delV=V2-V1;  //Change of the volume in L
```

```

W=-P*delV*101.3;  //Work done in the irreversible gas expansion in J

q=-W;  //Work done in the irreversible gas expansion change into heat lost by surrounding in J

qsur=-q;  //Heat lost by surrounding in J

T=293; //Temperature of the gas in K

delSsur=qsur/T;  //Entropy change for the surrounding in J K^-1

printf("\nEnropy change for the surrounding = %.1f J K^-1",delSsur);

delSuniv=delSsys+delSsur;  //Entropy change for the Universe in J K^-1

printf("\nEntropy change for the universe = %.1f J K^-1",delSuniv);
```

Scilab code Exa 5.5 Calucate the Entopy change for Fusion and Vaporization

```
//Calucate the Entopy change for Fusion and Vaporization

//Example 5.5

clc;

clear;
```

```

delfusH=6.01;  //Molar Enthalpy of fusion in kJ mol^-1

Tf=273;  //Melting point of ice in K

delfusS=(delfusH*1000)/Tf;  //Entropy change for fusion in J K^-1 mol^-1

printf("Entropy change for Fusion = %.1f J K^-1 mol^-1",delfusS);

delvapH=40.79;  //Molar enthalpy of vaporization in kJ mol^-1

Tb=373;  //Boiling point of water in K

delvapS=(delvapH*1000)/Tb;  //Entropy change for vaporization in J K^-1 mol^-1

printf("\Enentropy change for Vaporization = %.1f J K^-1 mol^-1",delvapS);
```

Scilab code Exa 5.6 `Calculate the increase in Entropy at consant pressure`

```


//Calculate the Increase in Entropy at constant pressure

//Example 5.6

clc;
```

```

clear;

m=200;  //Mass of water in g

M=18.02;  //Molar mass of water in g mol^-1

n=m/M;  //Number of moles of water present in mol

t1=10;  //Initial temperature of water in degree Celsius

T1=10+273;  //Initial temperature of water in K

t2=20;  //Final temperature of water in degree Celsius

T2=20+273;  //Final temperature of water in K

delCpbar=75.3;  //Molar heat capacity of water at constant pressure in J K^-1

delS=(n*delCpbar)*log(T2/T1);  //Increase in Entropy at constant pressure in J K^-1

printf("Increase in Entropy = %.1f J K^-1",delS);
```

Scilab code Exa 5.7 Calculate the change in Entopy for System Surounding and Unive

```
//Calculate the change in Entopy for System , Surounding and Universe when supercooled water turning into ice at -10degcelcious and 1atm pressure
```

```

//Example 5.7

clc;

clear;

n=2;  //Number of moles of water in mol

Cbarp1=75.3;  //Molar heat capacity of water at -10 degcelcious in J K^-1 mol^-1

T2=273;  //Temperature of water in K

T1=263;  //Temperature of supercooled water in K

delS1=(n*Cbarp1)*log(T2/T1);  //Change in Entropy when supercooled water change into loquid water in J K^-1

Cbarp2=22;  //Molar heat capacity of ice at 273 K in J K^-1 mol^-1

delS2=-n*Cbarp2;  //Change in Entropy when water change into ice in J K^-1

Cbarp3=37.7;  //Molar heat capacity of ice at 263 K in J K^-1 mol^-1

delS3=(n*Cbarp3)*log(T1/T2); //Entropy change when ice change into -10degcelcious of ice

delSsys=delS1+delS2+delS3; //Entropy change for the system in J K^-1

printf("Entropy change for the system = %.1f J K^-1",delSsys);

```

```
delT=T2-T1;  //Change in temperature in K

qsur1=-n*Cbarp1*delT;  //Heat lost by surrouding when supercooled water change in liquid water in J

delHfus=6.01*1000;  //Molar Enthalpies of fusion of water in J mol^-1

qsur2=n*delHfus;  //Heat given off to the surrouding when water freezes at 273 k in J

qsur3=n*Cbarp3*delT;  //Heat release to the surrouding when ice is cooloing from 273 K to 263 K in J

qsurtotal=qsur1+qsur2+qsur3;  //Total heat change in surrouding in J

delSsur=(qsurtotal/T1)/1.026;  //Change in Entropy for surrouding at 263 K in J K^-1(/1.03 is f0r taking delSsur to one decimal)

printf("\nEntropy change for surrouding = %.1f J K^-1",delSsur);

delSuniv=delSsys+delSsur;  //Entropy change for universe in J K^-1

printf("\nEntropy change for universe = %.1f J K^-1",delSuniv);
```

Scilab code Exa 5.8 Calculate the value of the Standard molar Entropy of the react

```
//Calculate the value of the Standard molar Entropy of the reactions (a)CaCO3(s)gives CaO(s)+CO2(g).(b)2H2(g)+O2(g)gives 2H2O(l).(c)N2(g)+O2(g)gives 2NO(g)

//Example 5.8

clc;

clear;

Sbar1=39.8;  //Standard Molar Entropy of CaO in J K^-1 mol^-1

Sbar2=213.6;  //Standard Molar Entropy of CO2 in J K^-1 mol^-1

Sbar3=92.9;  //Standard Molar Entropy of CaCO3 in J K^-1 mol^-1

delrS1=(Sbar1+Sbar2)-(Sbar3);  //Standard Molar Entropy change for the reaction (a)in J K^-1 mol^-1

printf("(a)Standard Molar Entropy change for Calcium Carbonate = %.1f J K^-1 mol^-1",delrS1);

Sbar4=69.9;  //Standard Molar Entropy of H2O in J K^-1 mol^-1

Sbar5=130.6;  //Standard Molar Entropy of H2 in J K^-1 mol^-1

Sbar6=205.0;  //Standard Molar Entropy of O2 in J K^-1 mol^-1

delrS2=(2*Sbar4)-((2*Sbar5)+(Sbar6)); //Standard Molar Entropy change for the reaction (b)in J K
```

```
   ^-1 mol^-1

printf(”\n (b)Standard Molar Entropy change for
   Hydrogen = %.1f J K^-1 mol^-1”,delrS2);

Sbar7=210.6;  //Standard Molar Entropy of NO in J K
   ^-1 mol^-1

Sbar8=191.5;  //Standard Molar Entropy of N2 in J K
   ^-1 mol^-1

Sbar9=205.0  //Standard Molar Entropy of O2 in J K
   ^-1 mol^-1

delrS3=(2*Sbar7)-((Sbar8)+(Sbar9));  //Standard
   Molar Entropy change for the reaction (c)in J K
   ^-1 mol^-1

printf(”\n (c)Standard Molar Entropy change for
   Nitrogen = %.1f J K^-1 mol^-1”,delrS3);
```

Scilab code Exa 5.9 `Calculate the Entropies change for the System Surrouding and U`

```
//Calculate the Entropies change for the System ,
   Surrouding and Universe for the reaction N2(g)+3
   H2(g)=2NH3(g)

//Example 5.9

clc;

clear;

```

```
Sbar1=192.5;  //Standard Molar Entropy of NH3 in J K^-1 mol^-1

Sbar2=191.5;  //Standard Molar Entropy of N2 in J K^-1 mol^-1

Sbar3=130.6;  //Standard Molar Entropy of H2 in J K^-1 mol^-1

delSsys=(2*Sbar1)-((Sbar2)+(3*Sbar3));  // Entropy change for the system in J K^_1 mol^-1

printf("Entropy change of the System = %.0f J K^-1 mol^-1",delSsys);

T=298;  //Temperature in K

delHsys=-92.6;  //Enthalpy change of the system in kJ mol^-1

delHsur=-delHsys;  //Enthalpy change for the surroundind  in kJ mol^-1

delSsur=(delHsur*1000)/T;  //Entropy change for the surrouding in J K^_1 mol^-1

printf("\nEntropy chnage for the Surrouding = %.0f J K^-1 mol^-1",delSsur);

delSsur1=311;  //Entropy change for the surrouding in J K^_1 mol^-1(delSsur1=delSsur)

delSuniv=delSsys+delSsur1;  //Entropy change for the universe in J K^_1 mol^-1

printf("\nEntropy chnage for the Universe = %.0f J K^-1 mol^-1",delSuniv);
```

Chapter 6

Gibbs and Helmholtz Energies and Their Applications

Scilab code Exa 6.1 `How much of energy change can be extracted as work in the meta`

```
//How much of energy change can be extracted as work in the metabolism of glucose to water and carbon dioxide C6H12O6(s)+6O2(g)=6CO2(g)+6H2O(l)

//Example 6.1

clc;

clear;

T=298;  //Teperature in K

delrU=-2801.3;  //Change in Enternal energy in kJ mol^-1

delrS=260.7;  //Change in Entropy in J K^-1

delrA=delrU-(T*delrS/1000);  //Change in Helmholtz Energy that can be used in amount of work done in
```

```
given process in kJ mol^-1

printf("Amount of work done = %.1f kJ mol^-1",delrA);
```

Scilab code Exa 6.2 `Calculate the value of Change in Gibbs Energy delG for melting`

```
//Calculate the value of Change in Gibbs Energy (delG) for melting of ice at 0 degree celcious, 10 degree celcious and minus 10 degree celcious

//Example 6.2

clc;

clear;

delH=6.01;  //Change in Enthalpy in kJ mol^-1

T1=273;  //Temperature of ice in K

delS=22.0;  //Change in Entropy in J K^-1

delG1=delH-(T1*delS/1000);  //Change in Gibbs Energy in kJ

printf("(a)Change in Gibbs Energy at Zero degree celcious = %.0f ",delG1);

T2=283;  //Temperature of ice in K

delG2=delH-(T2*delS/1000);  //Change in Gibbs Energy in kJ
```

```

printf("\n(b)Change in Gibbs Energy at Ten degree celcious = %.2f kJ",delG2);

T3=263;  //Temperature of ice in K

delG3=delH-(T3*delS/1000);  //Change in Gibbs Energy in kJ

printf("\n(c)Change in Gibbs Energy at minus Ten degree celcious= %.2f kJ",delG3);
```

Scilab code Exa 6.3 `Calculate the Maximum Electrical work that can be obtained fro`

```
//Calculate the Maximum Electrical work that can be obtained from CH4(g)+2O2(g)=CO2(g)+2H2O(l)

//Example 6.3

clc;

clear;

delrH=-890.3;  //change in Enthalp in kJ mol^-1

delrS=-242.8;  //Change in Entropy in J K^-1

T=25+273;  //Temperature in K

delrG=delrH-(T*delrS/1000);  //Change in Gibbs energy in kJ mol^-1

Welmax=delrG;  //Change in Gibbs Energy converted
```

```
   into maximum electrical work in kJ mol^-1 thus
   the maximum electrical work the system can do on
   the surroundings is equal to positive

printf("Maximum work done = %.0f kJ mol^-1",Welmax);
```

Scilab code Exa 6.4 `Calculate the Change in Gibbs Energy`

```
//Calculate the Change in Gibbs Energy

//Example 6.4

clc;

clear;

P1=1.50;   //Initial pressure in bar

P2=6.90;   //Final pressure in bar

n=0.590;   //Number of mole of sample in mol

T=300;   //Temperature of the gas in K

R=8.314;   //Gas constant in J K^-1 mol^-1

delG=(n*R*T)*log(P2/P1);   //Gibbs energy in J

printf("Change in Gibbs Energy = %.2f *10^3 J",delG
   *10^-3);
```

Scilab code Exa 6.5 `Calculate the slope of the S L solid liquid Curve`

```
//Calculate the slope of the S-L (solid -liquid ) Curve

//Example 6.5

clc;

clear;

Tf=273.15;  //Phase transition temperature (two phase can coexist in equilibrium)in K

delfusHbar=6.01*1000*9.87*10^-3;  //Change in Enthalpy in L atm mol^-1 (1 J=9.87*10^-3 L atm)

Vbarl=0.0180;  //Molar volume of liquid water in L mol^-1

Vbars=0.0196;  //Molar volume of ice in L mol^-1

delfusVbar=(Vbarl-Vbars);  //Change in molar volume in L mol^-1

F=(delfusHbar)/(Tf*delfusVbar);  //Slope of the S-L curve in atm K^-1; F=delP/delT

printf("Slope of the S-L Curve = %.0f atm K^-1",F);
```

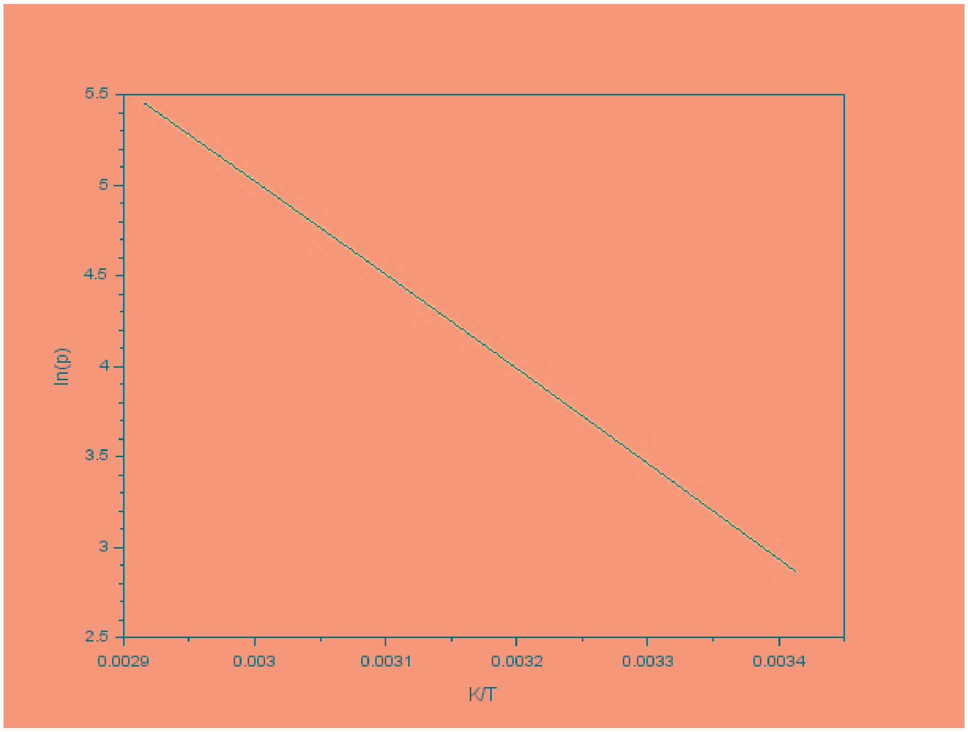

Figure 6.1: Determine the Molar Enthalpy of vaporization for water

Scilab code Exa 6.6 `Determine the Molar Enthalpy of vaporization for water`

```
//To calculate the Molar Enthalpy of Vapourisation

//Example 6.6

clc;

```

```
clear;

T=[20,30,40,50,60,70];

p=[17.54,31.82,55.32,92.51,149.38,233.7];

for i=1:6
    x(i)=1/(T(i)+273);
end

for i=1:6
    y(i)=log(p(i));
end

plot(x,y);

xlabel("K/T", "fontsize", 2);//Putting the x-axis as K/T

ylabel("ln(p)", "fontsize", 2);//Putting the y-axis as ln(Kp)

m=-(y(2)-y(1))/(x(2)-x(1));

R=8.314;

delH=R*m/1000;

printf("Molar Enthalpy of Vapourization of Water = %.1f kJ mol^-1",delH);
```

Chapter 7

Nonelectrolyte Solutions

Scilab code Exa 7.1 `Calculate the Gibbs Energy and Entropy of mixing of Argon and`

```
//Calculate the Gibbs Energy and Entropy of mixing of Argon and Nitrogen

//Example 7.1

clc;

clear;

n1=1.6;  //Number of moles of Argon at 1 atm

n2=2.6;  //Number of moles of Nitrogen at 1 atm

XAr=n1/(n1+n2);  //The mole fraction of Argon and Nitrogen

XN2=n2/(n1+n2); // The mole fraction of Nitrogen and Argon

n=n1+n2;  //Total moles of gas in mol

```

```
R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;  //Temperature of the gas

delmixG=n*R*T*(XAr*log(XAr)+XN2*log(XN2))/1000;  //The Gibbs Energy of mixing in kJ

printf("Gibbs Energy of mixing = %.1f kJ",delmixG);

delmixS=-(delmixG*1000)/T;  //Entropy of mixing in J K^-1

printf("\nEntropy of mixing = %.0f J K^-1",delmixS);
```

Scilab code Exa 7.2 `Calculate the Composition of the Vapor in Equilibrium of Liqui`

```
//Calculate the Composition of the Vapor in Equilibrium of Liquid A and Liquid B

//Example 7.2

clc;

clear;

XA=36/100;  //Number of mole of Liquid A

XB=1-(36/100);  //Number of mole of liquid B

PdegA=66;  //Vapor pressure of pure A in torr

PdegB=88;  //Vapor pressure of pure B in torr

```

```
PA=XA*PdegA;  //Vapor pressure of A in solution in
   torr

PB=XB*PdegB;  //Vapor pressure of B in solution in
   torr

PT=PA+PB;  //Total Vapor pressure of solution in
   torr

XAv=PA/PT;  //Composition of Vapor of A in solution

printf("Composition of Vapor of A = %.2f ",XAv);

XBv=PB/PT;  //Composition of Vapor B in solution

printf("\nComposition of Vapor of B = %.2f",XBv);
```

Scilab code Exa 7.3 Caculate the Molal Solubility of Carbon di Oxide in water

```
//Caculate the Molal Solubility of Carbon Dioxide in
    water

//Example 7.3

clc;

clear;

Pco2=3.3*10^-4*760;  //Partial pressure of CO2 in
   air in torr

K=1.24*10^6;  //Henry's Law Constant in torr

```

```
Xco2=Pco2/K;  //Mole raction of solue (CO2)

nH2O=1000/18.01;  //Mole fraction of solvent (H2O)in mol^-1

nCO2=Xco2*nH2O;  //Molal solubility of CO2 in mol/kg (H2O)

printf("Molal Solubility of Carbon di Oxide = %.2f*10^-5 mol/kg",nCO2*10^5);

Kdes=29.3;  //Henry's Law Constant in atm mol^-1 kg^-1

m=(Pco2/760)/Kdes;  //Molal solubilty of CO2 in mol/kg(H2O)(Alternatively we can find out )(The answer vary  due to round off error)

printf("\nMolal solubility = %.2f*10^-5 atm mol^-1 kg^-1",m*10^5);
```

Scilab code Exa 7.4 `Calculate the Boiling point and freezing poin of solution of S`

```
//Calculate the Boiling point and freezing poin of solution of  Sucrose in water

//Example 7.4

clc;

clear;

m1=45.20;  //Mass og the Sucrose in g
```

```

m2=316.0/1000;  //Mass 0f the water in kg

n=m1/342.3;  // Molar mass of the Sucrose in mol

Kb=0.51;  //Molal boiling point Elevation constant in K kg mol^-1

m3=n/m2;  //Molality of the solution in mol kg^-1

delT1=(Kb*m3)+373.15;  //Boiling point for solution of Sucrose in water

printf("(a)Boiling point of Sucrose = %.2f K",delT1);

Kf=1.86;  //Molal freezing point depression constant in K kg mol^-1

delT2=273.15-(Kf*m3);  //Boiling point for solution of Sucrose in water

printf("\n(b)Freezing point of Sucrose = %.2f K",delT2);
```

Scilab code Exa 7.5 `What is the Molar mass of Hemoglobin`

```
//What is the Molar mass of Hemoglobin

//Example 7.5

clc;

```

```
clear;

h=77.8/1000;  //Height Of the liquid in right column
    in m

g=9.81;  //Acceleration due to gravity in m s^-2

rho=1*10^3;  //Density of the solution in kg m^-3

P=h*g*rho;  //Osmotic pressure of the solution in
   pascals (N m^-2)

R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;  //Temperature of the solution in K

c2=20;  //Concentration of the solute in kg m^-3

mew2=(c2*R*T)/P;  //Molar mass of the Hemoglobin in
   kg mol^-1

printf("Molar mass of Hemoglobin = %.0f kg mol^-1",
   mew2);
```

Chapter 8

Electrolyte solutions

Scilab code Exa 8.1 `Calculate the Specific conductance`

```
//Calculate the Specific conductance

//Example 8.1

clc;

clear;

C=0.689;   //Cunductance of the cell in ohm^-1

c=0.255;   //Cell constant in  cm^-1 (c=l/A)

k=C*c;  //Specific conductance in ohm^-1 cm^-1

printf("Specific conductance = %.3f ohm^-1 cm^-1",k);
```

Scilab code Exa 8.2 `Calculate the Equivalent Conductance of NaCl solution`

```
//Calculate the Equivalent Conductance of NaCl solution

//Example 8.2

clc;

clear;

c1=0.0560;  //Molar concentration of KCl in solution mol L^-1

equiV1=134.5;  //Equivalent coductance of KCl in ohm^-1 equiv^-1 cm^2

k1=(equiV1*c1)/1000;  //Specific conductance of the KCl solution in ohm^-1 cm^-1

C1=0.0239;  //Conductance of the solution containing KCl in ohm^-1

c2=k1/C1;  //Cell constant of the solution in cm^-1

C2=0.0285;  //Conductance of the solution containing KCl and NaCl in ohm^-1

k2=c2*C2;  //Specific coductance of the NaCl solution ohm^-1 cm^-1

c3=0.0836;  //Molar concentration of NaCl in solution in mol L^-1

equiV2=(1000*k2)/c3;  //Equivalent conductance of NaCl in ohm^-1 equiv^-1 cm^2

printf("Equivalent Conductance = %.1f ohm^-1 equiv
```

```
^-1 cm^2",equiV2);
```

Scilab code Exa 8.3 `Calculate the Dissociation Constant of Acetic acid in given so`

```
//Calculate the Dissociation Constant of Acetic acid in given solution

//Example 8.3

clc;

clear;

c=0.10;  //Concentration of Acetic acid in mol L^-1

equiV=5.2;  //Equivalent conductance of Acetic acid in given concentration in equiv^-1 cm^2

equiVo=390.71;  //Equivalent conductance of Acetic acid at Infinite Dilution  in equiv^-1 cm^2

Ka=((c)*(equiV)^2)/((equiVo)*(equiVo-equiV));  //Dissociation constant of Acetic acid

printf("Dissociation constant = %.1f*10^-5 mol L^-1",Ka*10^5);
```

Scilab code Exa 8.4 `Calculate the Equivalent Conductance of Chloride ion at infini`

```
//Calculate the Equivalent Conductance of Chloride ion at infinite dilution ,How long it will take for the ion to travell between two electrodes

//Example 8.4

clc;

clear;

Uneg=7.91*10^-4;  //Mobility of Chloride ion in cm^2 s^-1 V^-1

F=96500;  //Faraday's constant in C mol^-1

Lemdaneg=F*Uneg;  //Equivalent conductance of the ion at infinite dilution in C s^-1 V^-1 mol^-1 cm^2 (ohm^-1 mol^-1 cm^2 or ohm^-1 equiv^-1 cm^2)

printf("(a)Equivalent Conductance = %.1f ohm^-1 equiv^-1 cm^2",Lemdaneg);
E=20;  //Electric field in V cm^-1

Vneg=E*Uneg;  //Ionic velocity of the ion in cm s^-1

d=4;  //Distance between two electrodes in cm

t=(d/Vneg)/60;  //Time taken by an ion to travel between two electrode in min

printf("\n(b)Time taken = %.1f min",t);
```

Scilab code Exa 8.5 Calculate the force in Newtons between a pair of Sodium positi

```
//Calculate the force in Newtons between a pair of Sodium positive ion and Chloride negative ion in vacuum and in water

//Example 8.5

clc;

clear;

QNa=1.602*10^-19;  //Charge on the Na ion in C

QCl=-1.602*10^-19;  //Charge on the Cl ion in C

Epsio=8.854*10^-12;  //Permittivity of the vacuum in C^2 N^-1 m^-2

r=1*10^-9;  //Distance between ions in m

F1=(QNa*QCl)/((4*%pi*Epsio)*(r)^2);  //Force in between a pair of ion in N

printf("(a)Force Between ions in vacuum = %.2f*10^-10 N",F1*10^10);

Epsi=78.54;  //Dielectric constant of water

F2=(QNa*QCl)/((4*%pi*Epsio*Epsi)*(r)^2);  //Force in between a pair of ion in water in N

printf("\n(b)Force between ions in water = %.2f*10^-12 N",F2*10^12);
```

Scilab code Exa 8.6 Calculate the value of Standard Molar Enthalpy of formation of

```
//Calculate the value of Standard Molar Enthalpy of formation of Sodium ion (delfHNa)for reaction Na(s)+1/2Cl2(g)=Na^+(aq)+Cl^-(aq)

//Example 8.6

clc;

clear;

delrH=-406.9;  //Standard Enthalpy of reaction in kJ mol^-1

delfH2=-167.2;  //Standard molar Enthalpy of Chloride ion in kJ mol^-1

delfH3=0;  //Standard molar Enthalpy of Chlorine gas in kJ mol^-1

delfH4=0;  //Standard molar Enthalpy of Sodium in kJ mol^-1

delfH1=delrH+delfH3+delfH4-delfH2;  //Standard molar Enthalpy of Sodium  ion in kJ mol^-1

printf("Standard Molar Enthalpy of Sodium ion = %.1f kJ mol^-1",delfH1);
```

Scilab code Exa 8.7 Expression for Chemical Potential of Magnesium Phosphate

```
//Expression for Chemical Potential of Mg3(PO4)2
```

```

//Example 8.7

clc;
clear;

v1=3;

v2=2;

v=5;

mv=((v1^v1)*(v2^v2))^(1/v);

printf("mu(Mg3(PO4)2) = mu0(Mg3(PO4)2)+ %.0f",v);

printf("RTln(%.2fm)",mv);
```

Scilab code Exa 8.8 Write Expression for the activities of Pottasium Chloride Sodi

```

//Write Expression for the activities of Pottasium Chloride Sodium Chromate and Aluminium sulphate

//Example 8.8

clc;

clear;

vpos1=1;  //Number of cation of KCl

vneg1=1;  //Number of anion of KCl
```

```

v1=vpos1+vneg1;  //Total number of ions of KCl

m1=(1*vpos1+1*vneg1)*(1/v1);  //Mean ionic molality of KCl

a1=m1; //Mean ionic activity ofelectrolyte

printf("mu KCl = %f ",a1);

printf("(m^%.1f)",v1);

printf("*(gamma^%.1f)",v1);

vpos2=2;  //Number of cation of KCl

vneg2=1;  //Number of anion of KCl

v2=vpos2+vneg2;  //Total number of ions of KCl

a2=((2^vpos2)*(1^vpos2));  //Mean ionic molality of KCl

printf("\nmu Na2CrO4 = %.0f",a2);

printf("*(m^%f)",v2);

printf("*(gamma^%.1f)",v2);

vpos3=2;  //Number of cation of KCl

vneg3=3;  //Number of anion of KCl

v3=vpos3+vneg3;  //Total number of ions of KCl

a3=(2^vpos3*3^vneg3);  //Mean ionic molality of KCl

printf("\nmu Al2(SO4)3 = %.0f",a3 );
```

```
printf("*(m^%.1f)",v3);

printf("*(gamma^%.1f)",v3);
```

Scilab code Exa 8.9 Calculate the Mean Activity coefficient of Cupper Sulphate

```
//Calculate the Mean Activity coefficient of Cupper
   Sulphate

//Example 8.9

clc;

clear;

m1=0.010;  //Molarity of the solution in m

z1=2;  //Charge on cation

z2=-2;  //Charge on anion

I=(1/2)*((m1*z1^2)+(m1*z2^2));  //Ionic strength of
   the solution in m

gyma=10^(-0.509*abs(z1*z2)*sqrt(I));  //Mean
   Activity coefficien of CuSO4

printf("Mean Activity coefficient = %.3f",gyma);
```

Scilab code Exa 8.10 `Calculate the Vant Hoff factor and the Degree of dissociation`

```
//Calculate the Van't Hoff factor and the Degree of dissociation for Chalcium Chloride (CaCl2)

//Example 8.10

clc;

clear;

m1=0.01;  //Molarity of CaCl2 in mol

m2=0.01;  //Molarity of sucroce in mol

op1=0.605;  //Osmotic pressure of CaCl2 in atm

op2=0.224;  //Osmotic pressure of sucrose in atm

P1=op1;  //Actual number of partical in solution at equilibrium

P2=op2;  //Number of particals in solution before dissociatio

i=P1/P2;  //Van;t Hoff factor for CaCl2

printf("Vant Hoff factor = %.2f",i);

v1=1;  //Number of cation

v2=2;  //Number of anion
```

```

v=v1+v2;  //Total number of ions

alpha=(i-1)/(v-1);  //Dgree of dissociation

printf("\nDegree of dissociation = %.2f",alpha);
```

Chapter 9

Chemical Equilibrium

Scilab code Exa 9.1 `Calculate the Equilibrium constant for the reaction`

```
//Calculate the Equilibrium constant for the reaction  N2(g)+3H2(g)=2NH3(g)

//Example 9.1

clc;

clear;

delfG1=-16.6;  //Standard Gibbs Energy for NH3  in kJ mol^-1

delfG2=0;  //Standard Gibbs Energy for N2  in kJ mol^-1

delfG3=0;  //Standard Gibbs Energy for NH3  in kJ mol^-1

delrGo=2*delfG1-(delfG2+3*delfG3);  //Standard Gibbs Energy change for reaction  in kJ mol^-1

```

```
R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;  //Temperature in K

Kp=exp(-delrGo*1000/(R*T));  //Equilibrium constant for the reaction (Equilibrium constant for the reaction is given by Kp=(PNH3/Pdeg)^2/((PN2/Pdeg)*(PH2/Pdeg)^2 )

printf("Equilibrium constant = %.1f*10^5",Kp*10^-5);
```

Scilab code Exa 9.2 `Calculate the Standard Gibbs Energy change for the reaction`

```
//Calculate the Standard Gibbs Energy change for the reaction (delrG) N2(g)+3H2(g)=2NH3(g)

//Example 9.2

clc;

clear;

Po=(760*10^5)/(1.01325*10^5);  //Standard pressure of the gas in torr

PN2=190;  //Partial pressure of the N2 gas in torr

PH2=418;  //Partial pressure of the H2 gas in torr

PNH3=722;  //Partial pressure of the NH3 gas in torr

Kp=((PNH3/Po)^2)/((PN2/Po)*(PH2/Po)^3);  //Equilibrium constant for reaction
```

```

R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;  //Temperature of the gas in K

delrGo=-33.2*10^3;  //Standard Gibbs energy for the reaction J mol^-1

delrG=(delrGo+(R*T)*log(Kp))/1000;  //Standard Gibbs Energy change for the reaction in kJ mol^-1

printf("Standard Gibbs Energy Change = %.1f kJ mol^-1",delrG);
```

Scilab code Exa 9.3 `Calculate the Equilibrium constant for the reaction`

```
//Calculate the Equilibrium constant for the reaction 2H2(g)+O2(g)=2H2O(l)

//Example 9.3

clc;

clear;

delG1=-237.2; //Standard Gibbs enaergy for H2O in kJ mol^-1

delG2=0; //Standard Gibbs enaergy for H2 in kJ mol^-1

delG3=0;  //Standard Gibbs enaergy for O2 in kJ mol^-1
```

```

delG=2*delG1-2*delG2-delG3; //Standard Gibbs enaergy change for the reaction in kJ mol^-1

R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;   //Temperature in K

Kp=exp(-(delG*1000)/(R*T));  //Equilibrium constant

printf("Equilibrium constant = %.1f*10^83",Kp*10^-83);
```

Scilab code Exa 9.4 `To calculate the values of Enthalpy and Entropy of Reaction`

```
//To calculate the values of Enthalpy and Entropy of Reaction

//Example 9.4

clc;

clear;

T=[872,973,1073,1173];//Temperatures in Kelvin

Kp=[1.8*10^-4,1.8*10^-3,1.08*10^-2,0.0480];//Equilibrium Constant

for i=1:4
    x(i)=1/T(i);//Defining x-axis of the graph as x
```

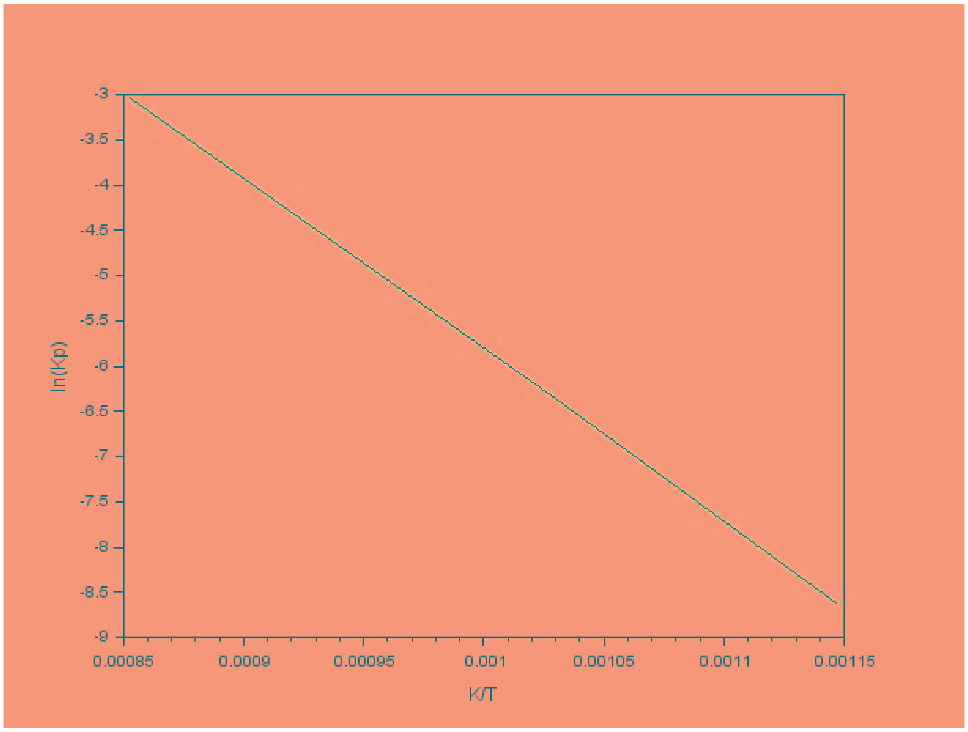

Figure 9.1: To calculate the values of Enthalpy and Entropy of Reaction

```
=1/T
end

for i=1:4
    y(i)=log(Kp(i));//Defining y-axis of the graph as y=log(Kp)
end

plot(x,y);//Plotting the Graph between 1/T and log(Kp)

xlabel("K/T", "fontsize", 2);//Putting the x-axis as K/T

ylabel("ln(Kp)", "fontsize", 2);//Putting the y-axis as ln(Kp)

m=-(y(2)-y(1))/(x(2)-x(1));//Slope of the Graph

R=8.314;//Universal Gas Constant in J K^-1 mol^-1

delH=R*m/1000;//Change in Enthalpy in kJ mol^-1

c=12.954;//y-Intercept of the Graph

delS=R*c;//Change in Entropy in J K^-1 mol^-1

printf("Change in Enthalpy of reaction = %.2f*10^2 kJ mol^-1",delH*10^-2);

printf("\n Entropy Change for the reaction = %.0f J K^-1 mol^-1",delS)
```

Scilab code Exa 9.5 `Calculate the values of change in Gibbs energy and Equilibrium`

```
//Calculate the values of change in Gibbs energy and Equilibrium constant  in biocchemical processes , Equilibrium constant for standard state .Also calculate the Gibbs energy change using both physical chemical standard state and biochemical standard state

//Example 9.5

clc;

clear;

R=8.314; //Gas constant in J K^-1 mol^-1

T=298; //Temperature in K

delG1=-21.8;  //Change in Gibbs energy in standard state in kJ mol^-1

K=exp((-delG1*1000)/(R*T));  //Equilibrium constant for standard state

printf("Equilibrium constant for standard = %.1f*10^3",K*10^-3);

delG2=delG1+39.93; //Change in Gibbs energy in biocchemical processes in kJ mol^-1

printf("\n Change in Gibbs energy in biocchemical processes =%.2f kJ mol^-1 ",delG2);

Kdes=exp(-(delG2*1000)/(R*T));  //Equilibrium constant  in biocchemical processes

printf("\n Equilibrium constant  in biocchemical
```

```
   processes = %.1f∗10ˆ−4”,Kdes*10^4);

C1=4.6*10^-3; //Concentration of NAD+ ion in M

C2=1.5*10^-2; //Concentration of NADH  in M

C3=3.0*10^-5; //Concentration of H+ ion in M

PH2=0.010;  //Standard pressure of H2 gas in bar

DelG1=((delG1*1000)+(R*T)*(log((C1*PH2)/(C2*C3))))
   /1000; //Gibbs energy change for Physical
   Chemical standard state in kJ molˆ−1

printf(”\n Gibbs energy change for Physical Chemical
    standard state = %.1f kJ molˆ−1 ”,DelG1);

DelG2=((delG2*1000)+(R*T)*(log((C1*PH2)/(C2*C3
   /10^-7))))/1000; //Gibbs energy change for
   Biochemists's Standard state in kJ molˆ−1

printf(”\n Gibbs energy change for Biochemists
   Standard state = %.1f kJ molˆ−1”,DelG2);
```

Chapter 10

Electrochemistry

Scilab code Exa 10.1 `Calculate the Equilibrium constant for the reaction And also`

```
//Calculate the Equilibrium constant for the reaction  Sn(s)+2Ag(one positive)(aq)=Sn(double positive)(aq)+2Ag(s).  And also predict whether the given reaction would occur spontaneously under standard-state condition

//Example 10.1

clc;

clear;

Ecathode=0.800;  //Standard Electrode Potential for Ag in V

Eanode=-0.138;  //Standard Electrode Potential for Sn in V

E=Ecathode-Eanode;  //Standard Electrode Potential for Electrochemical cell (positive quantity of E shows the reaction is spontaneous under standard-
```

```
state condition)

F=96500;  //Faraday costant in C mol^-1

v=2;  //Stoichiometric coefficient (two electron are transferred in reaction)

R=8.314;  //Gas constant in J K^-1 mol^-1

T=25+273;  //Temperature in K

K=exp((v*E*F)/(R*T));  //Equilibrium constant

printf("Equilibrium constant = %.1f*10^31",K*10^-31);

delrG=(-v*F*E)/1000;  //Gibbs Energy in kJ mol^-1 (large negative value of delrG indicate that the reaction is spontaneous under standard state condition)

printf("\n Spontaneity of the reactin = %.0f kJ mol^-1",delrG);
```

Scilab code Exa 10.2 `Calculate the Standard Reduction Potential for the Half react`

```
//Calculate the Standard Reduction Potential for the Half reaction Fe(three positive)(aq)+3 electron =Fe(s).

//Example 10.2

clc;
```

```

clear;

v1=2;  //Number of electron in first reaction

v2=1;  //Number of electron in second reaction

v3=3;  //Number of electron in third reaction

E1=-0.447;  //Standard Reduction Potential for first reaction in V

E2=0.771;  //Standard Reduction Potential for second reaction in V

E3=(v1*E1+v2*E2)/v3;  //Standard Reduction Potential for first reaction in V (delrG3=delrG1+delrG2)

printf("Standard Reduction Potential = %.3f V",E3);
```

Scilab code Exa 10.3 `Predict whether the following reaction would proceed spontane`

```
//Predict whether the following reaction would proceed spontaneously as written ( Cd(s)+Fe++(aq)=Cd++(aq)+Fe(s)

//Example 10.3

clc;

clear;

C1=0.15; //Concentration of Cadmium ion in M
```

```

C2=0.68;  //Concentration of Ferrus  ion in M

E1=-0.447; //Standard Electrode potential for cathode in V

E2=-0.403; //Standard Electrode potential for anode in V

Edes=E1-E2;  //Standard Electrode potential in V

v=2; //Stoichiometric coefficient

E=Edes-(0.0257/v)*log(C1/C2);  //Standard Electrode potential from Nerst equation in V

printf("Standard Electrode potential from = %.3f V is negative the reaction is not spontaneous as written",E);
```

Scilab code Exa 10.4 `Calculate the Equilibrium Constant for the reaction and the e`

```
//Calculate the Equilibrium Constant for the reaction and the emf of the cell

//Example 10.4

clc;

clear;

E1=1.72; //Standard Reduction Pontential for cathode in V
```

```

E2=0.771; //Standard Reduction Pontential for anode in V

Edes=E1-E2; //Standard Electrode Pontential for Electrochemical cell in V

F=96500;  //Faraday's constant in C mol^-1

v=1; //Stoichiometric coefficient

R=8.314;  //Gas constant in J K mol^-1

T=298;  //Temperature in K

K=exp((Edes*F*v)/(R*T));  //Equilibrium constant

printf("(a)Equilibrium constant = %.1f*10^16",K*10^-16);

C1=50.0*0.10/1000; //Number of moles of Fe ion initially present in mol

C2=10.0*0.10/1000; //Number of moles of Ce ion initially present in mol

V=0.060; //Total volume of the solution in L

x=2.3*10^-20; //Number of moles Ce at equilibrium in mol

C3=(C2-x)/V; //Number of moles of Ce plus 3 ion at equilibrium in mol

C4=(C2-x)/V; //Number of moles of Ferric ion at equilibrium in mol

C5=(C1-(C2-x))/V; //Number of moles of Ferrous 2
```

```
ion at equilibrium in mol

C6=x/V; //Number of moles of Ce plus 4  ion at equilibrium in mol

K1=(C3*C4)/(C6*C5); //Equilibrium constant

Edes1=0.771; //Standard Electrode  Pontential for Electrochemical cell in V

E=Edes1+0.0257*log(C4/C5); //emf of the  cell in V

printf("\n(b)emf of the cell = %.2f V",E);
```

Chapter 11

Acids and Bases

Scilab code Exa 11.1 `Calculate the concentration of the undissociated acid the H p`

```
//Calculate the concentration of the undissociated acid ,the H positive ion and the CN negative ion .And the percent dissociation

//Example 11.1

clc;

clear;

Ka=4.9*10^-10;  //Dissociatin constant of weak acid HCN at 298 K

x1=0.050;  //Concentration of HCN in M ,(HCN is a aweak acid assuming that at equilibrium the undissociated molecule of HCN is also same )

x=(Ka*x1)^(1/2);  //Concentration of H ion and CN ion at equilibrium in M (cocentration of both ion is equal)

```

```
printf("Concentration of ion = %.0f*10^-6 M",x*10^6);

x2=x1-x; //Concentration of undissociated acid at equilibrium in M

printf("\n Concentration of undissociated acid at equilibrium = %.3f M",x2)

X=(x/x1)*100;  //Percent dissociation of HCN

printf("\nPercent dissociation = %.0f*10^-2 percent",X*10^2);
```

Scilab code Exa 11.2 Monitoring the Titration

```
//Monitoring the Titration

//Example 11.2

clc;

clear;

Kin=4*10^-10;//Equilibrium Constant

pKin=-log10(Kin);//Negative Logarithm of Kin

phl=pKin-1;//Lower Value of pH

phu=pKin+1;//Upper Value of pH

printf("Phenophthalein can be used as an indicator
```

```
as it begins to change color from acid(colourless) at pH %f",phl);

printf("\nto base form (reddish pink)at pH %f",phu)
```

Scilab code Exa 11.3 `To Find the Concentrations of all the species in the reaction`

```
//To Find the Concentrations of all the species in the reaction

//Example 11.3

clc;

clear;

Ka=4.2*10^-7;//Acid Dissociation Constant for Carbonic Acid

Sol=1.1*10^-5;//Solubility of CO2 in equilibrium with water

a1=1;b1=Ka;c1=-Ka*Sol;//Coefficients a,b and c of the quadratic equation to find the concentration of H+

d1=(b1^2-(4*a1*c1));//Discriminant of the Quadratic Equation

x=(-b1+sqrt(d1))/(2*a1);//Concentration of H+

Ka2=4.8*10^-11;//Second Dissociation Constant for H2CO3
```

```

y=Ka2;//Concentration of CO3 2- ions

Kw=1*10^-14;//Disscociation Constant of Water

z=Kw/x;//Concentration of OH- ions (The answer vary due to round off error)

printf("At Equilibrium the concentrations are as follows:");

printf("\n [H+]=%.1f*10^-6 M",x*10^6);

printf("\n [OH-]=%.1f*10^-9 M",z*10^9);

printf("\n [H2CO3]=%.1f*10^-5 M",Sol*10^5);

printf("\n [HCO3-]=%.1f*10^-6 M",x*10^6);

printf("\n [CO3 2-]=%.1f*10^-11 M",y*10^11);
```

Scilab code Exa 11.4 Calculate the pH of of a buffer solution what is pH of the bu

```
//Calculate the pH of of a buffer solution what is pH of the buffer solution after the addition of HCl

//Example 11.4

clc;

clear;

```

```
C1=0.40; //Concentration of Acetic acid in M

C2=0.55; //Concentration of Sodium Acetate in M

pH1=4.76+log10(C2/C1); //pH of the Buffer solution before addition of HCl

printf("pH of the Buffer solution = %.2f",pH1);

C3=0.10; //Concentration of HCl in M

pH=4.76+log10((C2-C3)/(C1+C3)); // pH of the Buffer solution after addition of HCl

printf("\n pH of the Buffer solution after addition of HCl = %.2f",pH);
```

Scilab code Exa 11.5 Describe how you would prepare a phosphate buffer with a pH o

```


//Describe how you would prepare a phosphate buffer with a pH of seven point four

//Example 11.5

clc;

clear;

Ka1=7.5*10^-3; //Equilibrium constant for H3PO4= H++H2PO4-

```

```
pKa1=-log10(Ka1); //minus logarithm of Ka1

Ka2=6.2*10^-8; //Equilibrium constant for H2PO4-= H+ +HPO4--

pKa2=-log10(Ka2); //minus logarithm of Ka2

Ka3=4.8*10^-13; //Equilibrium constant for HPO4-- = H+ +PO3---

pKa3=-log10(Ka3); //minus logarithm of Ka3

pH=7.40; //pH of the required buffer solution

C1=10^(pH-pKa2); //Concentration of required solution to prepare buffer solution of  pH of 7.40

C=C1/1.0; //Ratio  of the required solution to prepare buffer solution of  pH of 7.40

printf("Ratio of the required solution = %.2f The buffer is dissolved to disodium hydrogen phosphate and sodium dihydrogen phosphate in a mole ratio of 1.5:1.0 ",C);
```

Chapter 12

Chemical Kinetics

Scilab code Exa 12.1 `To Calculate the rate Constant for the Reaction`

```
//To Calculate the rate Constant for the Reaction

//Example 12.1

clc;
clear;

t=[0,2000,4000,6000,8000,10000,12000];//Time in
   seconds

A=[1.5,1.26,1.07,0.92,0.81,0.72,0.65];//Absorbance

A0=1.5;//Absorbance at t=0s

Ainf=0.40;//Absorbance at t=infinity

for i=1:6
    x(i)=t(i);//Putting the x-axis as t/s
end
```

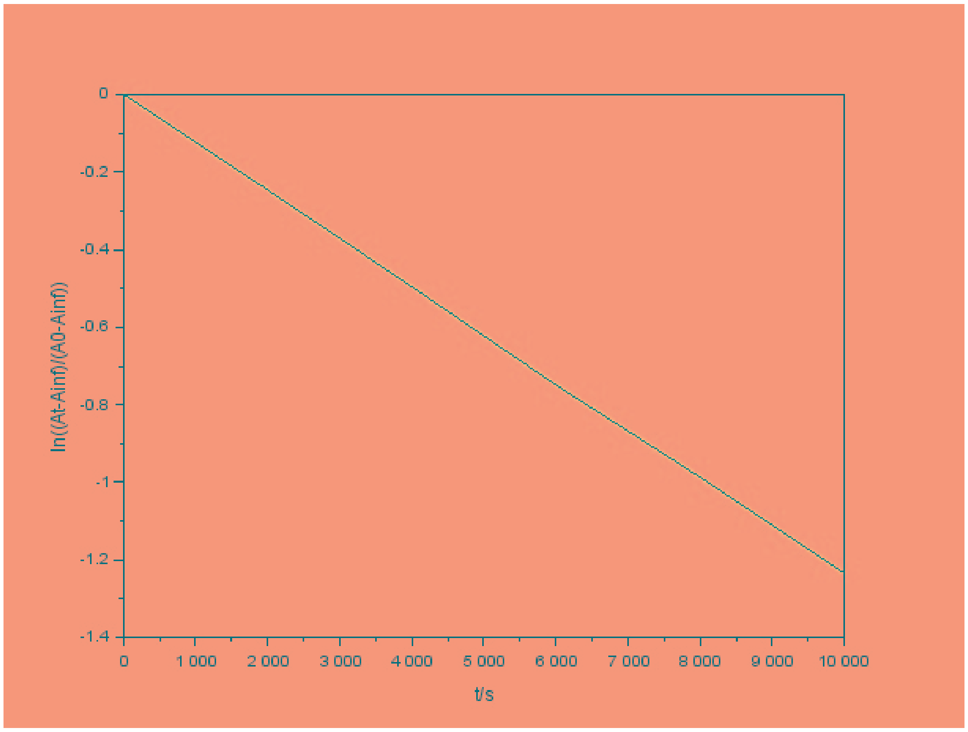

Figure 12.1: To Calculate the rate Constant for the Reaction

```

for i=1:6
    y(i)=log((A(i)-Ainf)/(A0-Ainf));//Putting the y-axis as ln((At-Ainf)/(A0-Ainf))
end

plot(x,y);//Plotting the Graph between x-axis and y-axis

xlabel("t/s", "fontsize", 2);//Putting the x-axis as t/s

ylabel("ln((At-Ainf)/(A0-Ainf))", "fontsize", 2);//Putting the y-axis as ln((At-Ainf)/(A0-Ainf))

m=-(y(2)-y(1))/(x(2)-x(1));//Calculating the slope (Rate Constant of Reaction) of Graph

printf("The rate constant for the reaction = %.3f *10^-4 s^-1",m*10^4);
```

Scilab code Exa 12.2 Calculate the standard molar Enthalpy of activation standard

```
//Calculate the standard molar  Enthalpy of activation (delH),standard molar Entropy of activation (delS)and Standard molar Gibbs energy of activation (delG) for the reaction CH3NC(g)=CH3CN(g)

//Example 12.2

clc;

```

```
clear;

k=4.0*10^13;  //Pre exponential factor in s^-1

KB=1.381*10^-23;  //Boltzman constant in J K^-1

h=6.626*10^-34;  //Planck's constant in J s

R=8.314;  //Gas constant in J K^-1 mol^-1

T=300;  //Absolute temperature in K

e=2.718;  //ln constant

delS=log((k*h)/(e*KB*T))*R;  // Standard molar Entropy in J K^-1 mol^-1

printf("Standard molar Entropy = %.2f J K^-1 mol^-1",delS);

Ea=272;  //Activation Energy in kJ mol^-1

delH=Ea-(R*T/1000);  //Standard molar Enthalpy in kJ mol^-1

printf("\n Standard molar Enthalpy = %.0f kJ mol^-1",delH);

delG=delH-(T*delS/1000);  //Standard molar Gibbs energy in kJ mol^-1(The answer vary due to round off error)

printf("\n Standard molar Gibbs Energy = %.3f kJ mol^-1",delG);
```

Scilab code Exa 12.3 `Estimate the Rate constant for a diffusion controlled reactio`

```
//Estimate the Rate constant for a diffusion controlled reaction in water

//Example 12.3

clc;

clear;

R=8.314;  //Gas constant in J K^-1 mol^-1

T=298;  //Absolute temperature in K

eta=8.9*10^-4;  //Viscosity of water in J s m^-3 (1J=1N m therefore N s m^-2=J s m^-3 )

KD=(8*R*T)*1000/(3*eta);  //Rate constant for diffusion controlled reaction in M^-1 s^-1(1 m^3 mol^-1 s^-1=1000 M^-1 s^-1)

printf("Rate constant for diffusion controlled reaction = %.1f*10^9 M^-1 s^-1",KD*10^-9);
```

Scilab code Exa 12.4 `Calculate the Rate constant for Forward abd Reverse reaction`

```
//Calculate the Rate constant for Forward abd Reverse reaction

//Example 12.4

clc;

clear

Tau=36*10^-6;  //The relaxation time for the system to reach the new equilibrium in s

C1=1.0*10^-7; //Concentration of the Hydrogen ion in M

C2=1.0*10^-7; //Concentration of the Hydroxyl ion in M (C1=C2)

C3=55.5;  //Concentration of the Water in M

Kf=C3/((Tau)*((C1+C2)*(C3)+(C1*C2)));//Rate constant for Forward reaction in M^-1 s^-1(Kf*C1*C2=Kr*C3)(Tau=1/(Kf*(C1+C2)+Kr)

printf("Rate constant for Forward reaction = %.1f*10^11 M^-1 s^-1",Kf*10^-11);

K=(C1*C2)/C3; //Equilibrium Constant for the reaction in M (Hydrogen ion +Hydroxyl ion=Water )

Kr=Kf*K; //Rate constant for Reverse reaction in s^-1

printf("\n Rate constant for Reverse reaction = %.1f*10^-5 s^-1 ",Kr*10^5);
```

Chapter 13

Enzyme Kinetics

Scilab code Exa 13.1 `To Determine the value of Km and Vmax of Enzyme and to Calcul`

```
//To Determine the value of Km and Vmax of Enzyme and to Calculate Kinetic Paramters imposed by inhibitors

//Example 13.1

clc;

clear;

s=[5*10^-4,1*10^-3,2.5*10^-3,5.0*10^-3,1.0*10^-2];//Substrate Concentration

v0no=[1.25*10^-6,2.0*10^-6,3.13*10^-6,3.85*10^-6,4.55*10^-6];//Initial Rate of an Enzyme Catalysed Concentration with no inhibitor

voA
```

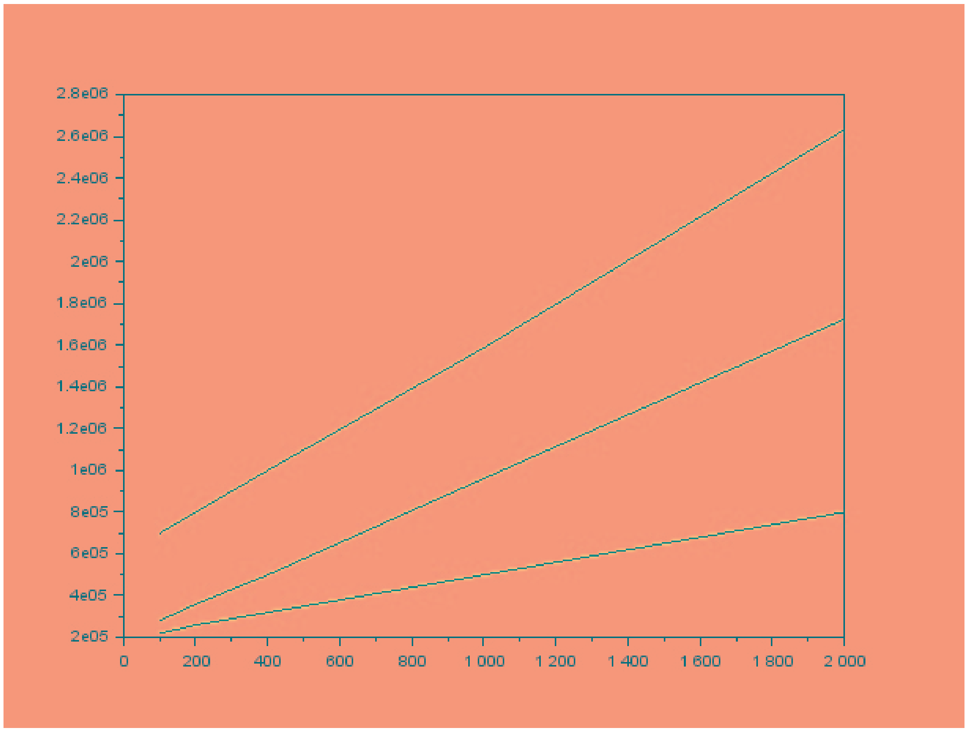

Figure 13.1: To Determine the value of Km and Vmax of Enzyme and to Calculate Kinetic Paramters imposed by inhibitors

```
=[5.8*10^-7,1.04*10^-6,2.00*10^-6,2.78*10^-6,3.57*10^-6];//Initial Rate of an Enzyme Catalysed Concentration with inhibitor A

voB=[3.8*10^-7,6.3*10^-7,1.00*10^-6,1.25*10^-6,1.43*10^-6];//Initial Rate of an Enzyme Catalysed Concentration with inhibitor B

for i=1:5
    Srec(i)=1/s(i);//Calculating the reciprocals of Substrate Concentrations
end

for i=1:5
    v0norec(i)=1/v0no(i);//Reciprocal of Initial Rate of an Enzyme Catalysed Concentration with no inhibitor
end

for i=1:5
    v0Arec(i)=1/voA(i);//Reciprocal of Initial Rate of an Enzyme Catalysed Concentration with inhibitor A
end

for i=1:5
    v0Brec(i)=1/voB(i);//Reciprocal of Initial Rate of an Enzyme Catalysed Concentration with inhibitor B
end

plot(Srec,v0norec);//Graph between Reciprocal of Substrate Concentration and Reciprocal of Initial Rate of an Enzyme Catalysed Concentration with no inhibitor

m1=(v0norec(2)-v0norec(1))/(Srec(2)-Srec(1));//Slope
```

```
of 1st Graph

vmax=1/(-m1*Srec(3)+v0norec(3));//Maximum Rate of reaction

Km=m1*vmax;//Maximum value of Kinetic Parameter

printf("The value of vmax=%.2f*10^-6 M s^-1",vmax*10^6);

printf("\nThe value of Km=%.1f*10^-3 M",Km*10^3)

plot(Srec,v0Arec);//Graph between Reciprocal of Substrate Concentration and Reciprocal of Initial Rate of an Enzyme Catalysed Concentration with inhibitor A

m2=(v0Arec(2)-v0Arec(1))/(Srec(2)-Srec(1));//Slope of 2nd Graph

I=8.0*10^-3;//Initial Concentration

K1=I/((m2*vmax/Km)-1);//Kinetic Parameter with Inhibitor A

printf("\nThe value of kinetic parameter with inhibitor A=%.1f*10^-3 M",K1*10^3)

plot(Srec,v0Brec);//Graph between Reciprocal of Substrate Concentration and Reciprocal of Initial Rate of an Enzyme Catalysed Concentration with inhibitor B

m3=(v0Brec(1)-v0Brec(3))/(Srec(1)-Srec(3));//Slope of 3rd Graph

K2=I/((m3*vmax/Km)-1);//Kinetic Parameter with Inhibitor B
```

```

printf("\nThe value of kinetic parameter with inhibitor B=%.1f*10^-3 M",K2*10^3)
```

Chapter 14

Quantum Mechanics and Atomic Structure

Scilab code Exa 14.1 `Calculate the Energy per mole of photon for the absorption of`

```
//Calculate the Energy per mole of photon for the absorption of blue ligght and red light

//Example 14.1

clc;

clear;

Lemda1=435*10^-9;   //Wavelength of blue light in m

h=6.626*10^-34;   //Planck's constant in J s

c=3.00*10^8; //Speed of light in m S^-1

E1=(h*c)/Lemda1;   //Energy of the photon for blue light in J

E2=(E1*6.022*10^23)/1000;   //Energy of blue light
```

```
for one mole of photon in kJ mol^-1

printf("Energy of blue light for one mole of photon = %.0f kJ mol^-1",E2);

Lemda2=680*10^-9;  //Wavelength of red light in m

E3=(h*c)/Lemda2;  //Energy of the photon for red light in J

E4=(E3*6.022*10^23)/1000;  //Energy of red light for one mole of photon in kJ mol^-1

printf("\n Energy of red light for one mole of photon = %.0f kJ mol^-1",E4);
```

Scilab code Exa 14.2 `Calculate radius of the smallest orbit of the Hydrogen atom`

```
//Calculate radius of the smallest orbit of the Hydrogen atom

//Example 14.2

clc;

clear;

Eo=8.8542*10^-12;  //Permittivity of free space in C^2 N^-1 m^-2

h=6.626*10^-34;  //Planck's constant in j s

Me=9.109*10^-31;  //Mass of the electron in kg
```

```

e=1.602*10^-19;   //Charge of an electron in C

n=1;   //Quantum number

Z=1;   //Atomic number of Hydrogen atom

r1=((n^2)*(h^2)*Eo)/((Z*%pi*Me)*(e^2));   //Radius of the Bohr orbit in m

r=r1/10^-10;   //Radius of the Bohr orbit in A

printf(”radius of the smallest orbit of the Hydrogen atom = %.3f A”,r);
```

Scilab code Exa 14.3 `Calculate the Wavelength in nanometer for transition in Hydro`

```
//Calculate the Wavelength in nanometer for transition in Hydrogen atom

//Example 14.3

clc;

clear;

nf=2;   //Quantum number for emmision process (n=4 to 2)

ni=4; //Quantum number for emmision process (n=4 to 20)

RH=109737;   //Rydberg constant in cm^-1
```

```

new=RH*abs((1/ni^2)-(1/nf^2));  //Frequency in cm^-1

Lemda1=1/new;  //Wavelength in cm

Lemda=Lemda1*10^7 //Wavelength in nm

printf("Wavelength = %.0f nm",Lemda);
```

Scilab code Exa 14.4 `Calculate the Wavelength associated with Tennis ball and for`

```
//Calculate the Wavelength associated with Tennis ball and for an Electron traveling at the same speed

//Example 14.4

clc;

clear;

h=6.626*10^-34;  //Planck's constant in J s

m1=6.0*10^-2;  //Mass of the tennis ball in kg

v=62;  ///Speed of the tennis ball in m s^-1

Lemda1=h/(m1*v);  //Wavelength of tennis ball in m (1 J=1 kg m^2 s^-2)

printf("Wavelength of tennis ball = %.1f*10^-34 m",Lemda1*10^34);

```

```
m2=9.10939*10^-31;  //Mass of the electron in kg

Lemda2=h/(m2*v);  //Wavelength of electron in m

Lemda=Lemda2*10^9;  //Wavelength of electron in nm

printf(”\n Wavelength of electron = %.1f*10^4 nm”,
   Lemda*10^-4);
```

Scilab code Exa 14.5 `What is a wavelength of an electron when it is accelerated`

```
//What is a wavelength of an electron when it is
   accelerated

//Example 14.5

clc;

clear;

h=6.626*10^-34;  //Planck's constant in J s

me=9.109*10^-31;  //Mass of the electron in kg

e=1.602*10^-19;  //Charge on an electron in C

V=1*10^3;  //Potencial difference in V

Lemda1=h/sqrt(2*me*e*V);  //Wavelength of an
   electron in m (1 J=1 C *1 V)

Lemda=Lemda1*10^9;  //Wavelength of  an electron in
   nm (1m=10^9 nm)
```

```
printf("Wavelength of an electron = %.4f nm",Lemda);
```

Scilab code Exa 14.6 `Calculate the uncertainty in the velocity of the electron and`

```

//Calculate the uncertainty in the velocity of the electron and Calculate the uncertainty in the baseball's position

//Example 14.6

clc;

clear;

delx=0.01*0.0529*10^-9;  //Uncertainty in the electron's posiion in m

h=6.626*10^-34;  //Planck's constant in J s

delp=h/(4*%pi*delx);  //Uncertaintty of momentum in kg m s^-1

m=9.1095*10^-31;  //Mass of the electron in kg

delv=delp/m;  //The uncertainty in the velocity in m s^-1

printf("(a)Uncertainty in the velocity = %.1f*10^8 m s^-1",delv*10^-8);

delp1=1*10^-7*6.7;  //Uncertainty in momentum in kg m s^-1
```

```

delx=h/(4*%pi*delp1);  //Uncertainty in the position in m

printf("\n(b)Uncertainty in the position = %.1f *10^-29 m ",delx*10^29);
```

Scilab code Exa 14.7 Calculate the Energy difference between the second orbital an

```
//Calculate the Energy difference between the second orbital and first orbital of the electron  and Calculate the Energy difference between the second orbital and first orbital for Nitrogen molucule

//Example 14.7

clc;

clear;

n1=1; //First quantum number

n2=2; //Second quantum number

m=9.109*10^-31; //Mass of the electron in kg

h=6.626*10^-34; //Planck's constant in J s

L1=0.10*10^-9; //Length of the box in m

E1=((n1^2)*(h^2))/(8*m*L1^2); //Energy for the enectron of first orbital in J
```

```

E2=((n2^2)*(h^2))/(8*m*L1^2); //Energy for the enectron of second orbital in J

E3=E2-E1; //Energy difference second orbital and first orbital in J

printf("(a)Energy difference second orbital and first orbital of the electron = %.1f*10^-17 J",E3*10^17);

m1=4.65*10^-26; //Mass of the Nitrogen molucule in kg

L2=10*10^-2; //Length of the box in m

E4=((n1^2)*(h^2))/(8*m1*L2^2); //Energy for the enectron of first orbital in J

E5=((n2^2)*(h^2))/(8*m1*L2^2); //Energy for the enectron of second orbital in J

E6=E5-E4; //Energy difference second orbital and first orbital in J

printf("\n(b)Energy difference second orbital and first orbital for Nitrogen molucule = %.1f*10^-40 J",E6*10^40);
```

Chapter 15

The Chemical Bond

Scilab code Exa 15.1 `Calculate the Percent Ionic character of the H F bond in Hydr`

```
//Calculate the Percent Ionic character of the H–F bond

//Example 15.1

clc;

clear;

mewexp=1.91*3.3356*10^-30;  //Experimental dipole moment in C m

Q=1.602*10^-19;  //Charge on electron in C

r=92*10^-12; //Distance between the ions in m

mewionic=Q*r;  //Dipole moment in C m

I=(mewexp/mewionic)*100;  //Percent Ionic character of the H–F bond in percent

```

```
printf("Percent Ionic character = %.1f percent ",I);
```

Scilab code Exa 15.2 `Calculate the Bond order of Nitric Oxide takes part in smog f`

```
//Calculate the Bond order of Nitric Oxide takes part in smog formation

//Example 15.2

clc;

clear;

MO=6; //Number of electron in bonding molecular orbital

AMO=1; //Number of electron in antibonding molecular orbital


BO=1/2*(MO-AMO); //Bond order of Nitric Oxide

printf("Bond order of Nitric Oxide = %.1f ",BO);
```

Scilab code Exa 15.3 `Calculate the Crystal Field Stabilization Energy CFSE`

```
//Calculate the Crystal Field Stabilization Energy (CFSE)

```

```
//Example 15.3

clc;

clear;

neg=0; //Number of electron in eg orbital

nt2g=5;  //Number of Electron in t2g orbital

CFSE=neg*0.6-nt2g*0.4; //Crystal Field Stabilization Energy (CFSE) in delta (crystal-field spliting)

printf("Crystal Field Stabilization Energy = %.1f delta",CFSE);
```

Chapter 16

Intermolecular Forces

Scilab code Exa 16.1 `Calculate the Dipole Dipole interaction energy in kJ mol inve`

```
//Calculate the Dipole-Dipole interaction energy in kJ mol^-1

//Example 16.1

clc;

clear;

mewA=1.08*3.3356*10^-30;  //Dipole moment in C m for one molecule

mewB=1.08*3.3356*10^-30;  //Dipole moment in C m for other molecule

epsilone=8.854*10^-12;  //Molar absorptivity or molar extinction coefficient in C^2 N^-1 m^-2

r=4*10^-10; //Distance between two molecule of HCl in m

```

```
V1=-(2*mewA*mewB)/(4*%pi*epsilone*(r)^3);  //Diploe-Diplole interaction in N m

V=(V1*6.022*10^23)/1000;  //Dipole-Dipole interaction in kJ mol^-1

printf("Dipole-Dipole interaction = %.1f kJ mol^-1 ",V);
```

Scilab code Exa 16.2 `Calculate the Potential Energy of Intraction in between Sodiu`

```
 //Calculate the Potential Energy of Intraction  in between Sodium ion and HCl molucule

//Example 16.2

clc;

clear;

mew=1.08*3.33*10^-30;  //Dipole moment in C m

r=4.0*10^-10; //Distance between Sodium ion and HCl molucule in m

epsilion=8.854*10^-12; //Molar absorption cofficient in C^2 N^-1 m^-2

q=1.602*10^-19; //Charge on electron in C

V1=-(q*mew)/(4*%pi*epsilion*r^2); //Potential energy of intraction in J

```

```
V=V1*6.023*10^23/1000; //Potential energy of intraction in kJ mol^-1

printf("Potential energy of intraction in between Sodium ion and HCl molucule = %.0f kJ mol^-1",V);
```

Scilab code Exa 16.3 `Calculate the Potential Energy of ion induced dipole intracti`

```
//Calculate the Potential Energy of ion induced dipole intraction  in between Sodium ion and Nitrogen  molucule

//Example 16.3

clc;

clear;

alpha=1.74*10^-30; //Proportionality constant in m^3

r=4.0*10^-10; //Distance between Sodium ion and Nitrogen molucule in m

epsilion=8.854*10^-12; //Molar absorption cofficient in C^2 N^-1 m^-2

q=1.602*10^-19; //Charge on electron in C

V1=-((1/2)*(alpha*q^2))/(4*%pi*epsilion*r^4); //Potential energy of ion induced dipole intraction in J

V=V1*6.023*10^23/1000; //Potential energy of ion
```

```
induced dipole intraction in kJ mol^-1

printf("Potential energy of ion induced dipole intraction in between Sodium ion and Nitrogen molucule = %.1f kJ mol^-1",V);
```

Scilab code Exa 16.4 Calculate the Potential Energy of Interaction between two Arg

```
//Calculate the Potential Energy of Interaction between two Argon atoms

//Example 16.4

clc;

clear;

alpha=1.66*10^-30; //Proportionality constant in m^3

I=1521; //Ionization energy of Argon in kJ mol^-1

r=4.0*10^-10; //Distance between two Argon atoms

V=-((3/4)*(alpha^2)*(I))/(r^6);  //Potential energy of interaction between two Argon atoms in kJ mol^-1

printf("Potential energy of interaction between two Argon atoms = %.2f kJ mol^-1",V);
```

Chapter 17

Spectroscopy

Scilab code Exa 17.1 `Calculate the bond length of Carbon monoxide`

```
//Calculate the bond length of Carbon monoxide

//Example 17.1

clc;

clear;

h=6.626*10^-34; //Planck's constant in J s

delv=1.15*10^11; //Frequency difference between two
   microwave spectrum of carbon monoxide

I=h/(4*(%pi^2)*delv); //Intensity of emerging light
   in kg m^2

m1=12.01; //Mass of the Carbon atom in amu

m2=16.00; //Mass of the Oxygen atom in amu

r1=(((I)*(m1+m2))/((m1*m2)*(1.661*10^-27)))^(1/2);
```

```
   //Bond length of CO in m

r=r1*10^10; //Bond length of CO in A

printf("Bond length of Carbon mono Oxide = %.2f A ",
   r);
```

Scilab code Exa 17.2 `Calculate the Force Constant of the HCl molucule`

```
//Calculate the Force Constant of the HCl molucule

//Example 17.2

clc;

clear;

c=3.00*10^10; //Speed of light in cm s^-1

newbar=2886; //Frequency in cm^-1

new=c*newbar; //Frequency in Hz

m1=1.008;  //Mass of the Hydrogen atom in amu

m2=34.97; //Mass of the Chlorine atom in amu

mew=(m1*m2*1.661*10^-27)/(m1+m2); //Reduced mass of
   the molucule in kg

K=4*%pi^2*new^2*mew; //Force constant of the
   molucule in N m^-1 (kg s^-2=kg m s^-2 m6-1, kg m
   s^-2 m^-1=N m^-1)
```

```

printf("Force constant of the molucule = %.2f*10^2 N m^-1",K*10^-2);
```

Scilab code Exa 17.3 `Calculate the Magnetic field that corresponds to a precession`

```
//Calculate the Magnetic field that corresponds to a precession frequency of 400 MHz

//Example 17.3

clc;

clear;

new=400*10^6; //Precession Frequency of Hydrogen atom in s^-1

gyma=26.75*10^7; //Gyromagnetic Ratio for Hydrogen atom in T^-1 s^-1 (T=Tesla)

Bo=(2*%pi*new)/gyma; //Magnetic field strength in T

printf("Magnetic field = %.2f T",Bo);
```

Chapter 18

Molecular Symmetry and Optical Activity

Scilab code Exa 18.2 `Calculate the Optical Rotation of Lysine solution What is the`

```
//Calculate the Optical Rotation of Lysine solution ,What is the difference between the Refractive indices of the left and right circularly polarized light and What is Molar Rotation of Lysine solution

//Example 18.2

clc;

clear;

c=0.148;  //Concentration of opticall active substance of L Lusine in g cm^-3

L1=10/10; //Length of the cell in dm

alpha1=+13.5;  //Specific rotation of L-Lssine in dm^-1 cm^3 g^-1 degree
```

```

alpha=alpha1*c*L1; //Optical Rotation of Lysine solution in degree (A positive alpha means that the plane of polarization is rotated to the right as one looks into the beam)

printf("(a)Optical Rotation of Lysine solution = +%.0f degree",alpha);

alpha2=+2; //The angle of rotation

lemda=589.3*10^-9; //Wavelength of light employed in m

L2=10/100; //Length of the cell in m

d=(alpha2*lemda)/(180*L2);  //Difference between the Refractive indices of the left and right circularly polarized light (d=nl-nr)

printf("\n(b)Difference between the Refractive indices of the left and right circularly polarized light = %.1f*10^-8",d*10^8);

alpha3=+13.5; //Specific rotation of L-Lysine solution in dm^-1 cm^3 g^-1

mew=146.2;  //Molar mass of L-Lysine solution in g mol^-1

fi=(alpha3*mew)/100; //Molar rotation of lysine solution in dm^-1 cm^3 mol^-1

printf("\n(c)Molar Rotation of Lysine solution = %.1f dm^-1 cm^3 mol^-1",fi);
```

Chapter 19

Photochemistry and Photobiology

Scilab code Exa 19.1 `Calculate the number of Einstens absorbed per second and the`

```
//Calculate the number of Einstens absorbed per second and the Total energy absorbed

//Example 19.1

clc;

clear;

A=0.65; //Absorbance of complex ion

epsilion=1.11*10^4; //Molar absorptivity or Molar extinction coefficient in L mol^-1 cm^-1

b=1; //Pathlength in cm

c1=A/(epsilion*b); //Concentraton in mol L^-1 or M

m=(c1*35)/1000; //number of moles of Ferrus ion
```

```
   produced in mol

q=0.93; //Quantum yield

fi=m/q; //Number of Einstens absorbed in mol or einstein

t=30*60;  //Time irradiated with monochromatic light in s

v=fi/t; //Rate of absorption in einstein s^-1

printf("Number of Einstens absorbed per second = %.1f*10^-9 einstein s^-1",v*10^9);

lemda=468*10^-9;  //Wavelength in m

c=3.0*10^8;  //Speed of light in m s^-1

new=c/lemda;  //Frequency of monochromatic light in s^-1

h=6.626*10^-34; //Planck's constant in J s

NA=6.022*10^23;  //Avogadro's number in mol^-1

E=fi*NA*h*new; //Energy absorbed in J

printf("\n Total Energy absorbed = %.2f J ",E);
```

Scilab code Exa 19.2 `Calculate the Partial pressure of Oxygen at an altitude of th`

```
//Calculate the Partial pressure of Oxygen at an altitude of 30 km (stratosphere)

//Example 19.2

clc;

clear;

Po=0.20; //Partial pressure of Oxygen at an sea level in atm

g=9.81; //Gravitational constant in m s^-2

h=30*10^3; //height in m

mew=0.03200; //Molar mass of Oxygen molucule in kg mol^-1

R=8.314; //Gas constant in J K^-1 mol^-1

T=25+273;  //Temperarure in K

P=Po*(exp(-(g*mew*h)/(R*T))); //Partial pressure of Oxygen at an altitude of 30 km (stratosphere)in atm

printf("Partial pressure of Oxygen at an altitude of 30 km = %.1f*10^-3 atm",P*10^3);
```

Chapter 20

The Solid State

Scilab code Exa 20.1 `To Calculate the smallest Diffraction Angle`

```
//To Calculate the smallest Diffraction Angle

//Example 20.1

clc;

clear;

a=2.6*10^-10;//Edge Length of Cubic Lattice

h=1;//Miller Indice h

k=1;//Miller Indice k

l=1;//Miller Indice l

lambda=1.542*10^-10;//Wavelength of light

theta=asin(lambda*sqrt(h^2+k^2+l^2)/(2*a))*180/%pi;

printf(”Smallest Diffraction Angle=%.1f degrees”,
```

```
theta);
```

Scilab code Exa 20.2 `Calculate the Lattice energy of Sodium Chloride`

```
//Calculate the Lattice energy of Sodium Chloride

//Example 20.2

clc;

clear;

n=8.4; //Integer between 8 and 12( For the repulsive term in the lattice)

NA=6.022*10^23; //Avogadro's number in mol^-1

mew=1.7476; //Madelung constant for the NaCl crystal lattice

e=1.602*10^-19; //Charge on electron in C

epsilion=8.854*10^-12 //Molar extinction cofficient in C^2 N^-1 m^-2

r=2.81*10^-10;  //Sum of radii of Sodium ion and Chlorine ion in m

Vbar=-((NA*mew*e^2)/(4*%pi*epsilion*r))*(1-(1/n)); //Lattice energy in J mol^-1(conversion factor 1J =1N m)

U=-Vbar/1000;  //Lattice energy in kJ mol^-1
```

```

printf("Lattice energy of Sodium chloride = %.0f kJ
    mol^-1",U);
```

Chapter 21

The Liquid State

Scilab code Exa 21.1 `How high will water rise in Xylem vessel of a plant`

```
//How high will water rise in Xylem vessel of a
   plant

//Examlpe 21.1

clc;

clear;

gyma=0.07275; //Suface tension in N m^-1

r=0.020*10^-2; //Radius of Xylem vessel in m

g=9.81; //Acceleration due to gravity in m s^-1

rho=1*10^3; //Density of water in kj m^-3

costheta=1; //Beacause the contact angle is quite
   small we assume that theta=0

h=(2*gyma*costheta)/(rho*g*r); //Height of the water
```

```
that rise up in Xylem vessel in m (1 N=1 kg m s^-2 therefore N s^2 kg^-1=1 m)

printf(" Hight of the  water that rise up in Xylem vessel of a plant = %.3f m",h);
```

Scilab code Exa 21.2 Calculate the Root Mean Square distance traveled by a urea mo

```
//Calculate the Root Mean Square distance traveled by a urea molucule

//Example 21.2

clc;

clear;

D=1.18*10^-9; //Diffusion coefficient of Urea in m^2 s^-1

t=1*60*60; //Diffusion time in second

meanx=sqrt(2*D*t)*1000; //Root mean square distance in mm

printf("Root mean square distance traveled = %.1f mm",meanx);
```

Scilab code Exa 21.3 Estimate the Diffusion Coeffcient of a spherical molucule

```
//Estimate the Diffusion Coeffcient of a spherical
    molucule

//Example 21.3

clc;

clear;

KB=1.381*10^-23; //Boltzmann's constant in J K^-1

T=300;  //Temperature in K

eta=0.00101; //Viscosity of the solvent in N s m^-2

r=1.5*10^-10; //Radius of molucule in m

D=(KB*T)/(6*%pi*eta*r); //Diffusion cofficient of a
    molucule in m^2 s^-1 (1 J N^-1 m s^-1=1 m^2 s^-1)

printf("Diffusion coeffcient of a spherical molucule
     = %.1f*10^-9 m^2 s^-1",D*10^9);
```

Chapter 22

Macromolecules

Scilab code Exa 22.1 `Calculate the molar mass of Catalase`

```
//Calculate the molar mass of Catalase

//Eaxmple 22.1

clc;

clear;

R=8.314;  //Gas constant in J K^-1 mol^-1

T=20+273;  //Temperature in K

D=4.1*10^-11; //Diffusion coefcient of Catalase (
   horse liver) in m^2 s^-1

rho=0.998; //Density of water in g ml^-1

s=11.3*10^-13; //Sedimentation coeffcient in s

vbar=0.715; //Partial specific volume in ml g^-1

```

```
mew=(s*R*T*1000)/((D)*(1-(vbar*rho))); //Molar mass of Catalase in g mol^-1 (1 J=1 kg m^2 s^-2)(The answer vary due to round off error )

printf("Molar mass of Catalase = %.2f*10^5 g mol^-1",mew*10^-5);
```

Chapter 23

Statistical Thermodynamics

Scilab code Exa 23.1 `Calculate the Partition function of the system`

```
//Calculate the Partition function of the system

//Example 23.1

clc;

clear;

KB=1.381*10^-23; //Boltzmann's constant in J K^-1

T=300; //Temperature in K

g0=1; //Degeneracies for zero level

g1=3; //Degeneracies for first level

g2=5; //Degeneracies for second level

e0=0; //Energy for zero level

e1=2.00*10^-21;  //Energy for first level in J
```

```
e2=8.00*10^-21; //Energy for second level in J

q=g0*exp((-e0)/(KB*T))+g1*exp((-e1)/(KB*T))+g2*exp((-e2)/(KB*T));  //Partition function of the system (The answer vary due to round off error )

printf("Partition function of the system = %.2f",q);
```

Scilab code Exa 23.2 `Calculate the Translational Partition function of a Helium at`

```
//Calculate the Translational Partition function of a Helium atom

//Example 23.2

clc;

clear;

m=4.003*1.661*10^-27; //Mass of Helium atom in kg amu^-1

KB=1.381*10^-23; //Boltzmann's constant in J K^-1

T=298; //Temperature in K

h=6.626*10^-34; //Planck's constant in J s

V=1; //Volume of container in m^3

Qtrans=(((2*%pi*m*KB*T)^(3/2))*V)/h^3;  //Translational Partition function of a Helium atom
```

```
(1 J=1 kg m^2 s^-2)

printf("Translational Partition function of a Helium atom = %.2f*10^30",Qtrans*10^-30);
```

Scilab code Exa 23.3 `Evaluate Vibrational Partition Function for Carbon Monoxide a`

```
//Evaluate Vibrational Partition Function for Carbon Monoxide at 300K and 3000K

//Example 23.3

clc;

clear;

h=6.626*10^-34;  //Planck's constant in J s

new=6.40*10^13;  //Fundamental frequency of vibration for CO in s^-1

KB=1.381*10^-23;  //Boltzmann's constant in J K^-1

T1=300; //Temperature in K

Qvib1=1/(1-exp((-h*new)/(KB*T1))); //Vibrational Partition Function for Carbon Monoxide at 300K

printf("Vibrational Partition Function for Carbon Monoxide at 300K = %.5f",Qvib1);

T2=3000; //Temperature in K

```

```
Qvib2=1/(1-exp((-h*new)/(KB*T2))); //Vibrational Partition Function for Carbon Monoxide at 3000K

printf(”\n Vibrational Partition Function for Carbon Monoxide at 3000K = %.2f”,Qvib2);
```