Scilab Textbook Companion for Thermodynamics: A Core Course by R. C. Srivastava, S. K. Saha And A. K. Jain[1]

Created by
Kedar Hanmant Kottawar
B.Tech
Chemical Engineering
VNIT , Nagpur (MH)
College Teacher
Shyam M Kodape
Cross-Checked by
Lavitha Pereira

May 24, 2016

---

[1] Funded by a grant from the National Mission on Education through ICT, http://spoken-tutorial.org/NMEICT-Intro. This Textbook Companion and Scilab codes written in it can be downloaded from the "Textbook Companion Project" section at the website http://scilab.in

Book Description

Title: Thermodynamics: A Core Course

Author: R. C. Srivastava, S. K. Saha And A. K. Jain

Publisher: PHI Learning Pvt. Ltd.

Edition: 2

Year: 2004

ISBN: 81-203-2498-6

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 2

Important Termonologies in Thermodynamics

Scilab code Exa 2.1 numerical

```
//example 2.1

clear;
clc;

//Given:
m=25;//weight of water vapour [grams]
w=18;//molecular weight of water vapour [grams/mol]
T=9.69;//increase in temperature [K]
Qp=0.45;//heat supplied at constant pressure[KJ]


//To find the molar constant pressure specific heat
n=m/w;//no. of moles of water vapour
Cp=Qp/(n*T);//specific heat capacity at constant pressure[KJ]
printf(”The specific heat capacity at constant pressure = %f KJ/K/mol”,Cp)
```

Scilab code Exa 2.2 numerical

```
//example 2.2

clear;
clc;

//Given:
m=16;//weight of oxygen [grams]
w=32;//molecular weight of oxygen [grams/mol]
T=300;//Temperature during compression [K]
P1=1;//initial pressure of process [atm]
P2=100;//final pressure of process[atm]
R=8.314;//Universal gas constant [J/K/mol]

//To find the minimum work of compression
n=m/w;//no. of moles of oxygen
W=-n*R*T*log(P1/P2);
printf("Mininmum work done to compress oxygen = %f J
    " , W )
```

Chapter 3

The First Law of Thermodynamics

Scilab code Exa 3.1 numerical

```
//example 3.1

clear;
clc;

//given:
V1=14;//initial volume of cylinder in m3
V2=9;//final volume of cylinder in m3
P=2000;//pressure during the operation in N/m2
U=(-6000);//internal energy of the system in J

//to find energy transfered in form of heat:
W=-P*(V2-V1);//work done during the operation in J
Q=U-W;//energy tranfered in form of heat in J
printf("energy tranfered in form of heat is %f J",Q)
  ;
```

Scilab code Exa 3.2 numerical

```
//example 3.2

clear;
clc;

//given:
R=8.314;//universal gas constant [J/K/mol]
T=300;//temperture for the process [K]
U=0;//change in internal energy [J]
V1=2.28;//initial volume [m3]
V2=4.56;//final volume[m3]


//to find the heat lost or gained by the system:
W=2.303*R*T*log10(V2/V1);//work done during the process[J]
Q=W;//heat lost or gained by the system[J]
printf(”the heat gained by the system is %f J”,Q);
```

Scilab code Exa 3.3 numerical

```
//example 3.3

clear;
clc;

//given:
H=29.2;//latent heat of vaporisation[KJ/mol]
T=332;//temperature of the system[K]
R=8.314;//universal gas constant [J/K/mol]


//to find Q,W,U for 1 mole of bromine vaporizes
```

```
//where Q is heat absorbed or evolved
//W is the work done by system
//U is the change in internak energy
Qp=H;//at constant pressure [KJ]
W=-R*0.001*T;//workdone [KJ]
U=Qp+W;//change in internal energy[KJ]
printf("heat absorbed by the bromine vapours is %f KJ",Qp);
printf("\nworkdone during the process is %f KJ",W);
printf("\nchange in internal energy of the system is %f KJ",U);
```

Scilab code Exa 3.4 numerical

```
//example 3.4

clear;
clc;

//given:
disp("C7H16(l) + 11O2(g) -> 7CO2(g) + 8H2O(l)");
n=-4;//change in no. of moles when reaction proceeds from reactants to products
T=298;//temperature of the process [K]
R=8.314;//universal gas constant [J/K/mol]
Qv=-4800;//heat energy at constant volume [KJ]


//to find change in enthalpy of the process:
U=Qv;//change in internal energy of system [KJ]
H=U+n*R*0.001*T;//change in enthalpy of the system[KJ]
printf("the change in enthalpy of system is %f KJ",H);
```

Scilab code Exa 3.5 numerical

```
//example 3.5

clear;
clc;

//given:
n=1;//number of moles of an given ideal gas
T=298;//temperature for the process[K]
V1=8.3;//initial volume of the ideal gas[m3]
V2=16.8;//final volume of the ideal gas[m3]
R=8.314;//universal gas constant[J/K/mol]


//to find the Q,W,H
//where Q is heat absorbed or evolved by the system
//W is the net workdone
//H is the change in enthalpy of system
W=-2.303*R*T*log10(V2/V1);//[J]
Q=-W;//[J]
disp("H=U+PV ,where U is change in internal energy
   which is zero due to isothermal process");
disp("PV where V is change in volume of system ,PV=
   RT & RT==0 since T i.e change in temp is zero for
    system");
disp("Therefore,the change in enthalpy is 0J");
printf("the workdone by system is %f J",W);
printf("\nthe heat evolved is %f J",Q);
```

Scilab code Exa 3.6 numerical

```
//example 3.6

clear;
clc;

//given:
T1=323;//intial temperature of water[K]
T2=373;//final temperature of water[K]
Cp=75.29;//specific heat of water[J/K/mol]
w=100;//weight of water[g]
mol.wt=18;//molecular weight of water[g/mol]

//to find the change in enthalpy(H) of water
n=w/mol.wt;//no. of moles of water[moles]
H=(n*Cp*(T2-T1))*0.001;//change in enthalpy of water [J]
printf("The change in enthalpy of water is %f J",H);
```

Scilab code Exa 3.7 numerical

```
//example 3.7

clear;
clc;

disp("SO2 + 0.5O2 -> SO3");
//given:
U=-97030;//heat of reaction[J]
n=1-(1+0.5);//change in no. of moles
R=8.314;//universal gas constant[J/K/mol]
T=298;//temperature during the reaction[K]


//to find the change in enthalpy of reaction(H)
H=U+n*R*T;//change in enthalpy of reaction[J]
```

```
printf("The change in enthalpy of reaction is %f J ",H);
```

Scilab code Exa 3.8 numerical

```
//example 3.8

clear;
clc;

disp("i.C(s) + O2(g) -> CO2(g)");
//Given:
H1=-393.5;//change in enthalpy [KJ/mol]
T1=298;//temperature [K]
n1=0;//change in no. of moles in reaction moving in forward direction
R=0.008314;//universal gas constant [KJ/K/mol]

//to find the change in internal energy (U) of given reaction
U1=H1-n1*R*T1;//change in internal energy [KJ]
printf("The change in internal energy is %f KJ/mol",U1);

disp("ii.C(s) + 0.5O2 -> CO(g)");
//Given:
H2=-110.5;//change in enthalpy[KJ/mol]
T2=298;//temperature[K]
n2=1-0.5;//change in no. of moles in reaction moving in forward direction
R=0.008314;//universal gas constant [KJ/K/mol]

//to find the change in internal energy (U) of given reaction
U2=H2-n2*R*T2;//change in internal energy [KJ]
```

```
printf("The change in internal energy is %f KJ/mol",U2);
```

Scilab code Exa 3.9 numerical

```
//example 3.9

clear;
clc;

disp("The standard heat of combustion of");
disp("2C6H6(l)+ 15O2(g)-> 12 CO2(g)+ 6 H2O(l)");
disp("H1(standard heat of combustion)=-6536 KJ/mol");
//Given:
H1=-6536;//standard heat of combustion [KJ/mol]

//to find the standard heat of rxn for combustion of 1 mole of C6H6
disp("C6H6(l)+ 7.5 O2(g)-> 6 CO2(g)+ 6 H2O(l)");
H2=H1/2;//standard heat of combustion[KJ/mol]
printf(" H2(standard heat of combustion for 1 mole of C6H6)= %f KJ/mol",H2);
```

Scilab code Exa 3.10 numerical

```
//example 3.10

clear;
clc;
disp("N2(g)+3H2(g)-> 2NH3(g)");

//Given:
```

```
H=-92.22;//standard heat of reaction [KJ/mol]

//to find the standard heat of formation of one mole of product
H1=H/2;//standard heat of formation of 1 mole [KJ/mol]
printf("H(heat of formation of 1 mole of product)=%f KJ/mol" , H1);
```

Scilab code Exa 3.11 numerical

```
//example 3.11

clear;
clc;

disp("C2H5OH(l)+3O2(g)->2CO2(g)+3H2O(l)");
//Given:
T=298;//temperature during the reaction[K]
Hw=-285.83;//standard heat of formation of liquid water [KJ/mol]
He=-277.69;//standard heat of formation of liquid ethanol[KJ/mol]
Hco2=-393.51;//standard heat of formation of carbon dioxide[KJ/mol]
Ho2=0;//standard heat of formation of oxygen gas[KJ/mol]

//to find the standard heat of reaction
H=2*Hco2+3*Hw-He-3*Ho2;//standard heat of reaction
printf("H(standard heat of reaction)=%f KJ/mol",H);
```

Scilab code Exa 3.12 numerical

```
//example 3.12

clear;
clc;

disp("CO(g)+NO(g)->0.5N2(g)+CO2(g)");
//Given:
Hrxn=-374;//standard heat of reaction[KJ/mol]
Hno=90.25;//standard heat of formation of NO[KJ/mol]
Hco2=-393.51;//standard heat of formation of CO2[KJ/mol]
Hn2=0;//standard heat of formation of N2[KJ/mol]
T=298;//temperature of reaction [K]

//to find the value of standard heat of formation of CO
Hco=0.5*Hn2+Hco2-Hno-Hrxn;//standard heat of formation of CO[KJ/mol]
printf("Hco(standard heat of formation)=%f KJ/mol",Hco);
```

Scilab code Exa 3.13 numerical

```
//example 3.13

clear;
clc;

//Given:
//("C3H6(g)+H2(g)->C3H8(g);H1=-29.6 Kcal");
//("C3H8(g)+5O2(g)->3CO2(g)+4H2O(l)   ;      H2=-530.6 Kcal");
//("C(s)+O2(g)->CO2(g);H3=-94.0 Kcal");
//("H2(g)+0.5O2(g)->H2O(l);H4=-68.3 Kcal. ");
H1=-29.6;//the standard heat of hydrogenation of
```

```
gaseous propylene to propane[Kcal]
H2=-530.6;//the heat of combustion of propane[Kcal]
H3=-94.0;//the heat of formation of carbon dioxide[Kcal]
H4=-68.3;//the heat of formation of liquid water[Kcal]


//to find the heat of combustion and formation of propylene
disp("C3H6(g)+4.5O2(g)->3CO2(g)+3H2O(l)");
H5=[3*H3+4*H4]-[H1+H2];//[Kcal]
printf("\n H(standard heat of combustion)=%f Kcal.\n",H5);
disp("3C(s)+3H2(g)->C3H6(g)");
H6=-H5+3*H3+3*H4;//[Kcal]
printf("\n H(standard heat of formation)=%f Kcal. \n",H6);
```

Scilab code Exa 3.14 numerical

```
//example 3.14

clear;
clc;

//Given:
H1=-114.1;//standard heat of reaction:2NO(g)+O2(g)->2NO2(g);[KJ/mol]
H2=-110.2;//standard heat of reaction:4NO2(g)+O2(g)->2N2O5(g);[KJ/mol]
H3=180.5;//standard heat of reaction:N2(g)+O2(g)->2NO(g);[KJ/mol]


```

```
//to find the heat of formation of N2O5
//reacton:N2(g)+2.5O2(g)->N2O5(g)
H4=(2*H1+H2+2*H3)/2;//standard heat of formation of N2O5[KJ/mol]
printf(”H(standard heat of formation of N2O5)=%f KJ/mol”,H4);
```

Scilab code Exa 3.15 numerical

```
//example 3.15

clear;
clc;

//Given:
Hc=-5645;//standard enthalpy of combustion of reaction:C12H22O11(s)+12O2(g)->12CO2(g)+11H2O(l)[KJ/mol]
Hf1=-393.51;//standard heat of formation of CO2: C(s)+O2(g)->CO2(g) [KJ/mol]
Hf2=-285.83;//standard heat of formation of H2O: H2(g)+0.5O2(g)->H2O(l) [KJ/mol]


//to find the standard heat of formaton of solid sucrose
//reaction:12C(s)+11H2(g)+5.5O2(g)->C12H22O11(s)
Hf=12*Hf1+11*Hf2-Hc;//[KJ/mol]
printf(”Hf(standard heat of formation of solid sucrose)=%f KJ/mol”,Hf);
```

Scilab code Exa 3.16 numerical

```
//example 3.16


clear;
clc;

//Given:
Hf1=-46.11;//standard heat of formation of NH3 at 298K //reaction:0.5N2(g)+1.5H2(g)->NH3(g) [KJ/mol]
Cp1=29.125;//molar heat capacity at constant pressure for N2(g)[J/K/mol]
Cp2=28.824;//molar heat capacity at constant pressure for H2(g)[J/K/mol]
Cp3=35.06;//molar heat capacity at constant pressure for NH3(g)[J/K/mol]
T1=298;//initial temperature[K]
T2=400;//final temperature[K]


//to find the standard heat of formation of NH3 at 400K for same reaction
Cp=Cp3-0.5*Cp1-1.5*Cp2;//[J/K/mol]
T=T2-T1;//[K]
Hf2=Hf1+Cp*0.001*T;//standard heat of formation for NH3 at 400K[KJ/mol]
printf("\n Hf2(standard heat of formation for NH3 at 400K = %f KJ/mol. \n",Hf2);
```

Scilab code Exa 3.17 numerical

```
//example 3.17

clear;
clc;
```

```

//Given:
Cp1=poly([29.07, -0.836*10^-3, 20.1*10^-7],'T','c');//heat capacity for H2(g)
Cp2=poly([25.72, 12.98*10^-3, -38.6*10^-7],'T','c');//heat capacity for O2(g)
Cp3=poly([30.36, 9.61*10^-3, 11.8*10^-7],'T','c');//heat capacity for H2O(g)
Hf1=-241820;//standard heat of formation H2O(g) at 298K :                    H2(g)+ 0.5O2(g)->H2O(g) [J/mol]
T1=298;//initial temperature[K]
T2=1273;//final temperature[K]

//to find the standard heat of formation of H2O(g) at 1273K
Cp=Cp3-0.5*Cp2-Cp1;//heat capacity for the formation [J/K/mol]
i=horner(Cp,1273)-horner(Cp,298);//[J/mol]
Hf2=(Hf1-i)*0.001;//[KJ/mol]
printf("The heat of formation of H2O at 1273K = %f KJ/mol", Hf2);
```

Scilab code Exa 3.18 numerical

```
//example 3.18

clear;
clc;

//given:
H1=435;//bond dissociation energy for: CH4->CH3+H [KJ/mol]
H2=364;//bond dissociation energy for:CH3->CH2+H [KJ/mol]
```

```
H3=385;//bond dissociation energy for:CH2–>CH+H [KJ/mol]
H4=335;//bond dissociation energy for:CH–>C+H [KJ/mol]


//to find the C–H bond energy of CH4 from the above bond energies
H=(H1+H2+H3+H4)/4;//the bond energy for C–H bond in CH4 [KJ/mol]
printf("\n H(the C–H bond energy in CH4)=%f KJ/mol.\n",H);
```

Scilab code Exa 3.19 numerical

```
//example 3.19

clear;
clc;

//Given:
H1=-84.68;//heat of formation : 2C(s)+3H2(g)–>C2H6(g) [KJ/mol]
H2=2*716.68;//heat of formation : 2C(s)–>2C(g) [KJ]
H3=3*436;//heat of formation : 3H2(g)–>6H(g) [KJ]
H4=412;//taking it as bond energy for one C–H bond[KJ/mol]


//to find the C–C bond energy in ethane bond
H=H2+H3-H1;//heat of reaction : C2H6(g)–>2C(g)+6H(g) [KJ/mol]
H5=H-6*H4;//bond energy for one C–C bond in ethane bond [KJ/mol]
printf("\n Hc–c(bond energy for one C–C bond in
```

```
   ethane bond)=%f KJ/mol.\n",H5);
```

Scilab code Exa 3.20 numerical

```
//example 3.20

clear;
clc;

//Given:
//MgBr2(s)-->Mg(s)+Br2(l)-->Mg(g)+Br2(l)-->Mg(g)+Br2
    (g)-->Mg(g)+2Br(g)-->Mg+2(g) + 2e(g) + 2Br(g)-->
   Mg+2(g) + 2Br-(g)
H1=-524;//enthalpy of formation of MgBr2(s) from its
     element [KJ/mol]
H2=148;//enthalpy of sublimation of Mg(s) [KJ/mol]
H3=31;//enthalpy of vaporization of Br2(l) [KJ/mol]
H4=193;//enthalpy of dissociation Br2 to 2Br(g) [KJ/
   mol]
H5=2187;//enthalpy of ionization of Mg(g) to Mg+2(g)
     [KJ/mol]
H6=-650;//enthalpy of formation of Br-(g) [KJ/mol]

//to find the lattice enthalpy of magnesium bromide
H=-H1+H2+H3+H4+H5+H6;//lattice enthalpy [KJ/mol]
printf("\n H(lattice enthalpy of magnesium bromide)=
   %f KJ/mol.\n",H);
```

Scilab code Exa 3.21 numerical

```
//example 3.21

clear;
```

```
clc;

//Given:
Cp1=poly([26.0, 43.5*10^-3, -148.3*10^-7],'T','c'); //heat capacity for CO2(g)[J/K/mol]
Cp2=poly([30.36, 9.61*10^-3, 11.8*10^-7],'T','c');//heat capacity for H2O(g)[J/K/mol]
Cp3=poly([27.30, -5.23*10^-3, -0.04*10^-7],'T','c'); //heat capacity for N2(g)[J/K/mol]
H1=-881.25;//heat of combustion of methane at 298K[KJ/mol]:                CH4 + 2O2(g) --> CO2(g) + 2H2O(l)
H2=43.6;//heat of vaporization of water at 298K[KJ/mol]:          H2O(l)-->H2O(g)
T1=298;//initial temperature [K]


//to find the maximum flame temperature when one mole of methane is burnt completely  in calculated amount of air(N2 to O2 ratio 4),at constant pressure
H=(H1+2*H2);//enthalpy of reaction: CH4 + 2O2(g) --> CO2(g) + 2H2O(g) [KJ]
printf("H(enthalpy of reaction)=%f KJ/mol.\n",H);
printf("H(enthalpy of heating)=%f KJ/mol. \n",-H);
Cp=Cp1+2*Cp2+8*Cp3;//[J/K/mol]
P=poly([0 , 305.12 , 52.28*10^-3 , -41.66*10^-7] , 'T' , 'c');
i=horner(P,298);
c1=-H*1000+i;
P1=poly([-c1 , 305.12 , 52.28*10^-3 , -41.66*10^-7] , 'T' , 'c');
T2=roots(P1)
printf("T2 (maximum flame temperature)= %f K",T2(1));
```

Chapter 4

Defining Thermodynamic State The State Postulate

Scilab code Exa 4.1 numerical

```
//example 4.1

clear;
clc;

//Given:
M=2.5;//mass of the substance[Kg]
x=0.6;//mass fraction for vapour phase
P=7;//pressure [atm]
T=438;//temperature[K]

//to find the mass of substance present in liquid and vapour phase
Ml=(1-x)*M;//mass fraction of liquid phase[Kg]
Mg=x*M;//mass fraction of vapour phase[Kg]

printf("M(liquid phase)=%f Kg , M(vapour phase)=%f Kg",Ml,Mg)
```

Scilab code Exa 4.2 numerical

```
//example 4.2

clear;
clc;

//Given:
Vl=0.0177;//specific volume of saturated liquid[m3/
    Kg]
Vg=4.43;//specific volume of saturated vapour[m3/Kg]
P=7;//pressure[atm]
T=438;//temperature[K]
x=0.6;//fraction of vapour phase
M=2.5;//mass of the substance[Kg]

//to find the total volume occupied by  the mixture
V=[(1-x)*Vl+x*Vg]*M;//total volume occupied [m3]
printf("Total volume occupied =%f m3", V)
```

Scilab code Exa 4.3 numerical

```
//example 4.3

clear;
clc;

//Given:
M=2.5;//mass of a substance[Kg]
x=0.6;//fraction of vapour phase
Ug=1105;//specific internal energy of saturated
    vapour[J/Kg]
```

```
Ul=298;//specific internal energy of saturated
    liquid[J/Kg]


//to find the total internal energy of the mixture
U=M*[(1-x)*Ul+x*Ug];
printf("The total internal energy of the mixture =
    %f J", U)
```

Chapter 5

The Second Law of Thermodynamics

Scilab code Exa 5.1 numerical

```
//example 5.1

clear;
clc;

//given:
T1=373;//initial temperature [K]
T2=573;//final temperature [K]
Q2=750;//Heat absorbed by carnot engine[J]

//to find the workdone , heat rejected , and
   efficiency of the engine
e=(T2-T1)/T2;//efficiency of the engine
W=e*Q2;//Workdone by the engine[J]
Q1=T1*Q2/T2;//Heat rejected by the engine[J]

printf("Efficiency of the engine = %f ", e);
printf("\n Workdone by the engine = %f J", W);
printf("\n Heat rejected by the engine = %f J", Q1);
```

Scilab code Exa 5.2 numerical

```
//example 5.2

clear;
clc;

//given:
T1=250;//temperature of heat rejection[K]
T2=1000;//temperature of heat absorption[K]

//to analyse the efficiency of the engine
e=1-(T1/T2);
printf(”Efficiency of the corresponding carnot engine = %f\n”,e);
disp(” Therefore , the inventors claim of 80% efficiency is absurd.The patent application should be rejected”);
```

Scilab code Exa 5.3 numerical

```
//example 5.3

clear;
clc;

//Given:
T1=323;//temperature [K]
T2=423;//temperature [K]
W=1.3;//work [KJ]

```

```

//To find the minimum heat required from heat source
    to yield the above work
e=(T2-T1)/T2;//efficiency
Q2=W/e;//minimum heat withdrawal from heat source[KJ
    ]
printf("Minimum heat withdrawal from heat source=%f
    KJ",Q2);
```

Scilab code Exa 5.5 numerical

```
//example 5.5

clear;
clc;
//Given:
T=298;//Temperature [K]
n=1;//no. of moles
V1=500;//initial volume [cm3]
V2=1000;//final volume [cm3]
R=8.314;//Universal gas constant [J/mol/K]

//to find the molar entropy change
S=R*log(V2/V1)//molar entropy change at constant
    temperature[J/K]
printf("Molar entropy change of argon = %f J/K", S);
```

Scilab code Exa 5.6 numerical

```
//example 5.6

clear;
clc;
```

```

//Given:
W=1728;//Isothermal and reversible work done[J/mol]
T=298;//Isothermal temperature[K]

//to find the change in molar entropy when the gas
   expands isothermally and reversibly

S=W/T;//change in molar entropy for isothermal and
   reversible process
printf("The change in molar entropy = %f J/mol/K", S
    );
```

Scilab code Exa 5.7 numerical

```
//example 5.7

clear;
clc;

//Given:
H=-92.22;//Standard reaction enthalpy[KJ]
T=298;//Temperature [K]


//To find the change in entropy of the surroundings
   at 298K
//standard reaction enthalpy is H.Therefore, heat
   gained by the surroundings at 298K is -H
S=-H*1000/T;//Change in entropy[J/K]
printf("Change in entropy of the surroundings at 298
   k = %f J/K",S);
```

Scilab code Exa 5.8 numerical

```
//example 5.8

clear;
clc;

//Given:
T1=298;//Initial Temperature[K]
T2=573;//Final Temperature[K]
Cv=29.1;//Specific Heat capacity of argon gas [J/K/mol]
n=1;//no. of moles


//To find the change in entropy for argon gas
S=n*Cv*log(T2/T1);//Change in entropy [J/K]
printf("The change in entropy of the argon gas is %f J/K",S);
```

Scilab code Exa 5.9 numerical

```
//example 5.9

clear;
clc;

//Given:
T1=276;//Initial temperature[K]
Tf=278.7;//Freezing point temperature[K]
Tb=353.3;//Boiling point temperature[K]
T2=373;//Final temperature[K]
Hf=9870;//Standard enthalpy of fusion[J/mol]
Hv=30800;//Standard enthalpy of vaporization[J/mol]
Cp=136.1;//Specific heat capacity of benzene[J/K/mol
```

```
]
mol.wt=78;//molecular weight of benzene[g/mol]
mass=200;//weight of solid benzene[g]
disp("     Cp doesnot change within this temp limit");

//To find the total entropy change of solid
n=mass/mol.wt;//no. of moles
S1=n*Cp*log(Tf/T1);//entropy change in heating [J/K]
S2=n*Hf/Tf;//entropy change in melting[J/K]
S3=n*Cp*log(Tb/Tf);//entropy change in heating[J/K]
S4=n*Hv/Tb;//entropy change in vaporization[J/K]
S5=n*Cp*log(T2/Tb);//entropy change in heating[J/K]
S=S1+S2+S3+S4+S5;//total entropy change in heating from 276 to 373K

printf("Total entropy change in heating 200g benzene from 3 to 100'C is %f J/K",S);
```

Scilab code Exa 5.10 numerical

```
//example 5.10

clear;
clc;

//Given:
mass=32;//weight of methane gas[gm]
P1=6*10^5;//Initial temperature[N/m2]
P2=3*10^5;//Final pressure[N/m2]
mol.wt=16;//molecular weight of methane gas[g/mol]
T=298;//Temperature[K]
//Isothermal process
R=8.314;//Universal gas constant[J/K/mol]

```

```
//To find the change in entropy of the gas
n=mass/mol.wt;//no. of moles
S=n*R*log(P1/P2);//change in entropy of gas[J/K]
printf("The change in entropy of the gas is %f J/K",
   S);
```

Scilab code Exa 5.11 numerical

```
//example 5.11

clear;
clc;

//Given:
N=3;//Total no. of balls
Nb=2;//Black balls
Nw=1;//white ball

//To find the total no. possible configuration
w=prod(1:N)/prod(1:Nb)/prod(1:Nw);

printf("The total no. of possible configurations are
    %f ",w);
```

Scilab code Exa 5.12 numerical

```
//example 5.12

clear;
clc;

//Given:
n=1;//no. of moles
```

```
T=273;//temperature [K]
Hf=6000;//enthalpy of fusion at 273K [J/mol]
k=1.38*(10^-23);//boltzmann constant[J/K]

//To find the relative number of distinguishable quantum states in 1 mole of water and ice at 273K

p=Hf/(k*T)/2.303;
w=10^(p);//w is the relative no. of distinguishable quantum states
printf("The relative no. of distinguishable quantum states in 1 mole of water and ice at 273K is %f",w);
```

Scilab code Exa 5.13 numerical

```
//example 5.13

clear;
clc;

//Given:
T=300;//temperature[K]
n=4;//no. of moles of an ideal gas
P1=2.02*10^5;//initial pressure[N/m2]
P2=4.04*10^5;//final pressure[N/m2]
R=8.314;//Universal gas constant[J/K/mol]

//To find the value of Gibb's free energy
G=n*R*T*log(P2/P1);//[J]
printf(" The change in Gibbs free energy is %f J",G);
```

Scilab code Exa 5.14 numerical

```
//example 5.14

clear;
clc;

//Given:
n=1;//no. of moles
T=300;//temperature[K]
V1=2;//initial volume[m3]
V2=20;//final volume[m3]
R=8.314;//Universal gas constant[J/K/mol]


//To find the work function or Helmholts free energy
A=-n*R*T*log(V2/V1);//Change in work function[J/mol]
printf("The change in Helmholts free energy is %f J/
   mol",A);
```

Scilab code Exa 5.15 numerical

```
//example 5.15

clear;
clc;

disp("C6H12O6(s) + 6O2(g) --> 6CO2(g) + 6H2O(l)");
//Given:
T=298;//Temperature[k]
R=8.314;//Universal gas constant[J/K/mol]
S=182.45;//standard entropy change at 298K [J/K]
U=-2808;//change in internal energy at 298K[KJ/mol]
//reaction is taking place in bomb calorimeter so no
    volume change
```

```
//therefore U=Q at constant volume

//To find the energy change that can be extracted as
    heat and work
A=U-T*S*0.001;//Energy extracted as heat[KJ/mol]
Wmax=A;//work done [KJ/mol]
dn=6-6;//change in no. of moles
H=U+dn*R*T;//Change in enthalpy of the bomb
   calorimeter[KJ]
printf("The energy change that can be extracted as
   heat is %f KJ/mol", A);
printf("\nThe energy change that can be extracted as
    work is %f KJ/mol", -A);
printf("\nThe change in enthalpy of bomb calorimeter
    is %f KJ/mol",H);
```

Scilab code Exa 5.16 numerical

```
//example 5.16

clear;
clc;

disp("C8H18(g)+12.5O2(g)-->8CO2(g)+9H2O(l)");
//Given:
T=298;//temperature[K]
S=421.5;//change in entropy[J/K]
H=-5109000;//Heat of reaction[J]
R=8.314;//Universal gas constant[J/K/mol]
dn=8-(1+12.5);//change in no. of moles


//To find the helmholts free energy and Gibbs free
   energy
U=H;//[J]
```

```
A=U-T*S;//Change in helmholts free energy[J]
G=A+dn*R*T;//Change in Gibbs free energy[J]
printf("The change in Helmholts free energy is %f J",A);
printf("\nThe change in Gibbs free energy is %f J",G);
```

Scilab code Exa 5.17 numerical

```
//example 5.17

clear;
clc;

disp("C3H6(g)+4.5O2(g)-->3CO2(g)+3H2O(l)");
//Given:
S=-339.23;//standard change in entropy [J/K]
T=298;//temperature[K]
Hf1=20.42;//enthalpy of formation of C3H6(g)[J]
Hf2=-393.51;//enthalpy of formation of CO2(g)[J]
Hf3=-285.83;//enthalpy of formation of H2O(l)[J]
dn=3-4.5-1;//change in no. of moles
R=8.314;//Universal gas constant[J/K/mol]

//To find the Helmholts free energy and Gibbs free energy
H=3*Hf2+3*Hf3-Hf1;//Enthalpy of the reaction[J]
U=H-dn*R*0.001*T;//Change in internal energy of the reaction[J]
A=U-T*S*0.001;//Helmholts free energy change[J]
G=A+dn*R*0.001*T;//Gibbs free energy change[J]
printf("The change in Helmholts free energy is %f J",A);
printf("\nThe change in Gibbs free energy is %f J ",G);
```

Scilab code Exa 5.19 numerical

```
//example 5.19

clear;
clc;

disp("CH4(g)+2O2(g)-->CO2(g)+2H2O(l)");

//Given:
S1=-242.98;//standard entropy change for the
    combustion reaction[J/K]
Hf1=-74.81;//Enthalpy of formation of CH4(g)[KJ/mol]
Hf2=-393.51;//Enthalpy of formation of CO2(g)[KJ/mol
    ]
Hf3=-285.83;//Enthalpy of formation of H2O(l)[KJ/mol
    ]
T=298;//temperature[K]

//To find the total entropy change
H=Hf2+2*Hf3-Hf1;//Change in enthalpy of reaction[KJ]
S2=-H*1000/T;//Change in entropy of the surrounding[
    J/K]
Stotal=(S1+S2)*0.001;//Total entropy change
printf("The total change in entropy is %f KJ/K",
    Stotal);
```

Scilab code Exa 5.20 numerical

```
//example 5.20

```

```
clear;
clc;

disp("2H2(g)+O2(g)-->2H2O(l)");
//Given:
Hf1=-285.83;//standard enthalpy of formation of H2O(l)[KJ/mol]
S=-327;//Standard entropy change for the same reaction[J/K]
T=298;//temperature[K]


//To find the spontanity of the reaction
H=2*Hf1-0-0;//Enthalpy of the reaction[KJ/mol]
G=H-T*S*0.001;//Change in Gibbs free energy[KJ]
printf("The change in Gibbs free energy is %f KJ\n ",G);
disp("As change in Gibbs free energy is negative. Therefore,the reaction is spontaneous")
```

Scilab code Exa 5.21 numerical

```
//example 5.21

clear;
clc;

disp("CH4(g)+2O2(g)-->CO2(g)+2H2O(l)");
//Given:
S=-242.98;//standard entropy change for reaction [J/K]
T=298;//temperature[K]
Gf1=-50.72;//standard Gibbs free energy of formation for CH4(g)[KJ/mol]
Gf2=-394.36;//standard Gibbs free energy of
```

```
formation for CO2(g)[KJ/mol]
Gf3=-237.13;//standard Gibbs free energy of formation for H2O(l)[KJ/mol]


//To find the standard enthalpy of reaction
G=Gf2+2*Gf3-Gf1;//Standard Gibbs free energy for reaction[KJ/mol]
H=G+T*S*0.001;//Standard enthalpy of reaction [KJ]
printf("The standard enthalpy of reaction is %f KJ",H);
```

Scilab code Exa 5.22 numerical

```
//example 5.22

clear;
clc;

disp("C6H12O6(s)+6O2(g)-->6CO2(g)+6H2O(l)");
//Given:
mass=25;//mass of glucose for combustion under standard condition[gm]
T=298;//temperature[K]
Gf1=-910;//Standard Gibbs free energy of formation for C6H12O6[KJ/mol]
Gf2=-394.4;//Standard Gibbs free energy of formation for CO2(g)[KJ/mol]
Gf3=-237.13;//Standard Gibbs free energy of formation for H2O(l)[KJ/mol]
mol.wt=180;//molecular weight of glucose[gm/mol]

//To find the maximum energy that can be extracted as non-expansion work is equal to the change in free energy of the system
```

```
G=6*Gf2+6*Gf3-Gf1
n=mass/mol.wt;//no. of moles
Gactual=G*n;//Gibbs free energy for the combustion of 0.139mol of glucose
printf("The energy that can be extracted as non-expansion work is %f KJ",-Gactual);
```

Scilab code Exa 5.23 numerical

```
//example 5.23

clear;
clc;

//Given:
a=1.39*10^-2;//constant for a vanderwaal's gas[lit2.atm/mol2]
b=3.92*10^-2;//constant for a vanderwaal's gas[lit2.atm/mol2]
R=0.082;//Universal gas constant[lit.atm/deg/mol]

//To find the value of the inversion temperature for the gas
Ti=(2*a)/(R*b);//inversion temperature [K]
printf("The inversion temperature for the gas is %f K",Ti);
```

Scilab code Exa 5.26 numerical

```
//example 5.26


clear;
```

```
clc;

//Given:
T=169.25;//Boiling point[K]
R=8.314;//Universal gas constant[J/K/mol]
disp("dlnP/dT=He/R*T^2");
disp("dlnP/dT=(2.303*834.13/T^2)+(1.75/T)-(2.30*8.375*10^-3)");
disp("Therefore using these two equations we calculate the He(enthalpy) of ethylene");

//To find the Enthalpy of vaporization of ethylene
x=(2.303*834.13/T^2)+(1.75/T)-(2.30*8.375*10^-3);//it is dlnP/dT
He=R*0.001*T^2*x;//Enthalpy of vaporization[J/mol]
printf("\n\nThe Enthalpy of vaporization of ethylene at its boiling point is %f KJ/mol",He);
```

Scilab code Exa 5.27 numerical

```
//example 5.27

clear;
clc;

//Given:
P1=101.3;//Initial Pressure[KPa]
P2=60;//Final Pressure[KPa]
He=31.8;//Enthalpy of vaporization[KJ/mol]
R=8.314;//Universal gas constant[J/K/mol]
T1=353.2;//boiling point of benzene at 101.3KPa[K]

//To find the boiling point of b/enzene at 60KPa
x=(T1^-1)-(R*0.001*log(P2/P1)/He);
T2=x^-1;//Boiling point of benzene at 60KPa
```

```
printf("The boiling point of benzene at 60KPa is %f K",T2);
```

Scilab code Exa 5.28 numerical

```
//example 5.28

clear;
clc;

//Given:
P1=0.016;//Vapour pressure of pure ethanol at 273K[bar]
P2=0.470;//Vapour pressure of pure ethanol at 333K[bar]
T1=273;//initial temperature [K]
T2=333;//final temperature[K]
R=8.314;//Universal gas constant[J/K/mol]
P=1.01;//vapour pressure at normal boiling point[bar]


//To find the molar enthalpy of vapourization
x=(T2^-1)-(T1^-1);
He=-R*0.001*log(P2/P1)/x;//molar enthalpy of vaporization[J/mol]
t=(T2^-1)-(R*0.001*log(P/P2)/He);
T=(t^-1)-273;//normal boiling point [C]
printf("The molar enthalpy of vapourization is %f J/mol",He);
printf("\n\nThe normal boiling point for pure ethanol is %f C",T);
```

Scilab code Exa 5.29 numerical

```
//example 5.29

clear;
clc;

//Given:
T2=353.2;//normal boiling point of benzene at
    1.01325bar[K]
T1=298;//temperature [K]
R=8.314;//Universal gas constant[J/K/mol]
P2=1.01325;//Vapour pressure of benzene[bar]
//benzene obey's Trouton's rule
disp(" from Troutons rule , ");
disp(" He/Tb=85J/K/mol");

//To find the vapour pressure of benzene at 298K
He=85*T2;//molar enthalpy of vapourization[J/K/mol]
x=(T2^-1)-(T1^-1);
t=-He*x/R;
P1=P2/exp(t);
printf("\nThe vapour pressure of benzene at 298K is
    %f bar",P1);
```

Scilab code Exa 5.30 numerical

```
//example 5.30

clear;
clc;

//Given:
c=1;//no. of components(only CO2)
p=2;//no. of phases(liquid + gas)
```

```

//To find the degrees of freedom
F=c-p+2;//degree of freedom
printf(”Degrees of freedom is %f \n\n”,F);
disp(”Degrees of freedom 1 means that either pressure or temperature can be varied independently,i.e.when temperature is fixed, pressure is automatically fixed”);
```

Scilab code Exa 5.31 numerical

```
//example 5.31

clear;
clc;

//Given:
c=1;//no. of components
p=1;//no. of phases

//To find the values of degrees of freedom
F=c-p+2;//Degrees of freedom
printf(”Degrees of freedom is %f\n\n”,F);
disp(”Degrees of freedom 2 means both the pressure and temperature can be varied independently”);
```

Scilab code Exa 5.32 numerical

```
//example 5.32

clear;
clc;

```

```
//Given:
P=1.75*10^-5;//Vapour pressure of pure water at 293K [torr]
dP=1.1*10^-7;//Lowering in vapour pressure of water
//To find the mole fraction of sucrose,so that the vapour pressure of water will be lowered by dP
x=dP/P;//mole fraction of sucrose
disp(x,'The mole fraction of sucrose is ');
```

Scilab code Exa 5.33 numerical

```
//example 5.33

clear;
clc;

//Given:
P=94.6;//The vapour pressure of pure benzene at 298K [torr]
n1=20;//no. of moles of pure benzene
n2=5;//no. of moles of pure naphthalene

//To find the partial vapour pressure of benzene over the solution
x=n1/(n1+n2);//(mole fraction of benzene)
p=x*P;//the partial vapour pressure of benzene[torr]
printf("The partial vapour pressure of benzene is %f torr",p);
```

Scilab code Exa 5.34 numerical

```
//example 5.34

```

```
clear;
clc;

//Given:
x=0.28;//mole fraction of solute
R=8.314;//Universal gas constant[J/K/mol]
T=298;//temperature[K]

//To find the reduction in chemical potential
du=R*T*log(1-x);//reduction in chemical potential[J/mol]
printf("The reduction in chemical potential is %f J/mol",-du);
```

Scilab code Exa 5.35 numerical

```
//example 5.35

clear;
clc;

//Given:
Kb=0.51;//ebullioscopic constant of water [K*Kg/mol]
n=155/180;//no. of moles of glucose
m=n/1;//[mol/Kg]
Ti=373;//Boiling point temperature of water[K]

//To find the boiling point of the solution which is made by dissolving 155g of glucose in 1000g of water
Tf=(Ti+Kb*m)-273;//boiling point temperature of the solution[C]
printf("The boiling point of the solution is %f C",Tf);
```

Scilab code Exa 5.36 numerical

```
//example 5.36

clear;
clc;

//Given:
Ti=5.44;//freezing point of pure benzene[K]
Tf=4.63;//freezing point of solution[K]
m1=2.12;//mass of the solute[gm]
m2=125;//mass of the benzene[gm]
Kf=5.12;//cryoscopic constant of pure benzene[K*Kg/
    mol]

//To find the molar mass of solute(M2)
dTf=Ti-Tf;//depression in freezing point[K]
M2=(m1*1000*Kf)/(m2*dTf);//molar mass of solute
printf("The molar mass of solute is %f",M2);
```

Scilab code Exa 5.38 numerical

```
//example 5.38

clear;
clc;

disp("N2(g)+3H2(g)<=>2NH3(g)");
//Given:
T=298;//Temperature[K]
Gf1=-16450;//Gibb's free energy of formation for NH3
    (g)[J/mol]
```

```
R=8.314;//Universal gas constant[J/K/mol]

//To find the Kp value of the above reaction
Gf=2*Gf1//Gibb's free energy for the reaction[KJ]
x=Gf/R/T
Kp=exp(-x);
disp(Kp,'The Kp for above reaction is ');
```

Scilab code Exa 5.39 numerical

```
//example 5.39

clear;
clc;

disp("0.5N2(g)+1.5H2(g)<=>NH3(g)");
//Given:
T=298;//Temperature[K]
Kp=900;//Equilibrium constant for above reaction
P1=0.32;//partial pressure of N2(g)[bar]
P2=0.73;//partial pressure of H2(g)[bar]
P3=0.98;//partial pressure of NH3(g)[bar]
R=8.314;//Universal gas constant[J/K/mol]

//To find the reaction Gibb's energy
G=-R*T*log(Kp);
x=(P1^0.5)*(P2^1.5);
p=P3/x;
Gr=(G+R*T*log(p))*0.001;
printf("The reaction Gibbs free energy is %f KJ/mol
    ",Gr);
```

Scilab code Exa 5.40 numerical

```
//example 5.40

clear;
clc;

disp(”N2(g)+3H2(g)<=>2NH3(g)”);

//Given:
Kp1=5.85*10^5;//equilibrium constant at 298K
H1=-46.11;//standard enthalpy of formation of NH3(g)[KJ/mol]
T1=298;//Initial temperature[K]
T2=423;//Final temperature[K]
R=8.314;//Universal gas constant[J/K/mol]

//To find the Kp at 423K temperature
H=2*H1;//enthalpy for reaction;[KJ]
t=(T1^-1)-(T2^-1);
x=-H*t/(R*0.001);
Kp2=Kp1*exp(x);
disp(Kp2,'The Equilibrium constant for reaction  at 423K is ');
```

Scilab code Exa 5.41 numerical

```
//example 5.41

clear;
clc;


disp(”Zn(s)|ZnCl2(aq)||CdSO4(aq)|Cd(s)”);
//For Zn(s)|ZnCl2(aq)||CdSO4(aq)|Cd(s)
//Given:
T=298;//Temperature[K]
```

```
R=8.314;//Universal gas constant[J/K/mol]
E1=-0.7618;//Standard electrode potential for Zn2+/Zn [volts]
E2=-0.403;//Standard electrode potential for Cd2+/Cd [volts]
F=96500;//Faraday's constant[coulomb/mol]
n=2;//no. of electrons balancing
//To find the Standard Free energy and equilibrium constant
Ei=E2-E1;//Standard potential for the reaction[volts]
Gi=-n*F*Ei;//Standard Gibb's Free Energy [KJ/mol]
Ki=exp(-Gi/R/T);//Equilibrium constant
printf("The Free energy for the rection is %f KJ/mol",Gi*0.001);
disp(Ki,'The value of equilibrium constant is ');


disp("Cd(s)|CdSO4(aq),Hg2SO4(s)|Hg(l)");
//For Cd(s)|CdSO4(aq),Hg2SO4(s)|Hg(l)
//Given:
E3=0.6141;//Standard electrode potential for Hg2SO4(s),SO4^2-/Hg(l) [volts]
//To find the standard free energy and equilibrium constant
Eii=E3-E2;//Standard potantial for the reaction[volts]
Gii=-n*F*Eii;//Standard Gibb's free energy[KJ/mol]
Kii=exp(-Gii/R/T);//Equilibrium constant
printf("The Free energy for the rection is %f KJ/mol",Gii*0.001);
disp(Kii,'The value of equilibrium constant is');
```

Scilab code Exa 5.42 numerical

```
//example 5.42

clear;
clc;

//Given:
disp("Zn(s)|ZnCl2(soln)||AgCl(s)|Ag–Ag|AgCl(s)|ZnCl2
   (soln)|Zn(s)");
m1=0.02;//concentration[M]
Y1=0.65;//mean ionic activity coefficient
m2=1.5;//concentration[M]
Y2=0.29;//mean ionic activity coefficient
R=8.314;//Universal gas constant[J/K/mol]
T=298;//Temperature [K]
F=96500;//Faraday's constant[coulomb/mol]

//To find the overall e.m.f of the above cell
E=R*T*(log(m2*Y2/m1/Y1))*3/2/F;//[volts]
printf("The overall e.m.f of the cell is %f volts",E
   );
```

Scilab code Exa 5.43 numerical

```
//example 5.43

clear;
clc;

//Given:
disp("H2(g,1atm)|HCl(aq)|HCl(aq)|H2(g,1atm)");
m1=0.02;//concentration[M]
Y1=0.88;//mean ionic activity coefficient
m2=1;//concentration[M]
Y2=0.81;//mean ionic activity coefficient
R=8.314;//universal gas constant[J/K/mol]
```

```
T=298;//Temperature[K]
F=96487;//Faraday's constant[coulombs/mol]
t=0.178;//Tranference number of Cl-1

//To find the e.m.f of the cell
E=-2*t*R*T*(log(m1*Y1/m2/Y2))/F;//e.m.f of the cell[volts]
printf("The e.m.f of the cell is %f volts",E);
```

Scilab code Exa 5.44 numerical

```
//example 5.44

clear;
clc;

disp("The values for reaction that goes on within the cadmium cell");
//Given:
n=2;//no. of moles
E=1.01463;//standard cadmium cell potential[volts]
d=-5*10^-5;//i.e d=dE/dT[V/K]
F=96500;//[coulomb/mol]
T=298;//Temperature [K]

//To find the values of dG,dS and dH
dG=-n*E*F;//Change in Gibb's free energy[J]
dS=n*F*d;//Change in entropy [J/K]
dH=dG+T*dS;//change in enthalpy[J]
printf(" dG=%f J",dG);
printf("\n dS=%f J/K",dS);
printf("\n dH=%f J",dH);
```

Chapter 6

The Question of Ideality

Scilab code Exa 6.2 numerical

```
//example 6.2

clear;
clc;

//Given:
T=500;//Temperature[K]
P=100;//Pressure[atm]
a=3.61;//van der waals constant for CO2[atm.L^2.mol
    ^-2]
b=0.0429;//van der waals constant for CO2[L.mol^-1]
R=0.082;//Universal gas constant[atm.K-1.mol^-1]

//To find the molar volume of CO2
x=b+(R*T/P);
y=a/P;
z=a*b/P;
p2 = poly([-z y -x 1], 'Vm', 'c');
t=roots(p2);
printf("The value of molar volume of CO2 is %f L.mol
    ^-1",t(3));
```

Scilab code Exa 6.5 numerical

```
//example 6.5

clear;
clc;

//Given:
b=0.0391;//Van der waals constant[dm3/mol]
R=0.082;//Universal gas constant[dm3*atm/mol]
P2=1000;//pressure [atm]
P1=0;//pressure [atm]
T=1273;//Temperature [K]

//To find the fugacity and fugacity coefficient
x=b*(P2-P1);
y=R*T;
fc=exp(x/y);//fugacity coefficient

f=P2*fc;//fugacity[atm]
printf("The fugacity is %f atm",f);
printf("\n The fugacity coefficient is %f ",fc);
```

Scilab code Exa 6.10 numerical

```
//example 6.10

clear;
clc;

//Given:
```

```
m1=0.03;//mass of CO2(g)[gm]
w1=44.01;//molecular weight of CO2(g)[gm/mol]
m2=250;//mass of water[gm]
w2=18.02;//molecular weight of water[gm/mol]
k=1.25*10^6;//Henry's law constant[Torr]
T=298;//Temperature[K]

//To find the partial pressure of CO2 gas
n1=m1/w1;//no. of moles of CO2
n2=m2/w2;//no. of moles of water
x1=n1/(n1+n2);//mole fraction of CO2
Pco2=k*x1;//Partial pressure of CO2[Torr]
printf(”The partial pressure of CO2 gas is %f Torr”, Pco2);
```

Scilab code Exa 6.11 numerical

```
//example 6.11

clear;
clc;

//Given:
W=1000;//Total mass of a solution[gm]
x1=0.5;//mole fraction of Chloroform
x2=0.5;//mole fraction of Acetone
V1m=80.235;//Partial molar volume of chloroform[cm3/mol]
V2m=74.166;//Partial molar volume of Acetone[cm3/mol]
M1=119.59;//molecular weight of chloroform[gm/mol]
M2=58;//molecular weight of Acetone[gm/mol]

//To find the Volume of the solution
nT=W/(x1*M1+x2*M2);//Total no. of moles
```

```
V=nT*(x1*V1m+x2*V2m);//Total volume[cm3]
printf("The volume of the solution is %f cm3",V);
```

Scilab code Exa 6.12 numerical

```
//example 6.12

clear;
clc;

//Given:
x1=0.5;//mole fraction of chloroform
x2=0.5;//mole fraction of p-xylene
T=298;//Temperature[K]
//to find the excess volume
Ve=x1*x2*[0.585+0.085*(x1-x2)-0.165*(x1-x2)^2];//Excess volume measured by using a dilatometer
printf("Ve/(cm3.mol^-1) = %f ",Ve);
```

Scilab code Exa 6.14 numerical

```
//example 6.14

clear;
clc;

//Given:
m1=0.01;//molality[m]
v11=1;
v12=2;
Y1=0.71;
m2=0.005;//molality[m]
v21=1;
```

```
v22=1;
Y2=0.53;


//To find the activity , molality of the electrolytes
v1=(v11)+(v12);
v2=(v21)+(v22);
a1=(m1^v1)*(v11^v11)*(v12^v12)*(Y1^v1);
a2=(m2^v2)*(v21^v21)*(v22^v22)*(Y2^v2);
x=1/v1;
a1m=a1^x;
m1m=m1*(v11^v11*v12^v12)^x;//molality[m]
y=1/v2;
m2m=m2*(v21*v21*v22^v22)^y;//molality[m]
a2m=a2^y;
disp(a1,'The activity of the electrolyte ZnCl2 is');
disp(a1m,'The mean activity of ZnCl2 is ');
disp(m1m,'The mean molality of ZnCl2 in [m] ');
disp(a2,'The activity of the electrolyte CuSO4 is ');
disp(a2m,'The mean activity of CuSO4 is ');
disp(m2m,'The mean molality of CuSO4 in [m] ');
```

Scilab code Exa 6.15 numerical

```
//example 6.15

clear;
clc;

//Given:
m2=3;//mass of the sucrose[gm]
m1=0.1;//mass of water [Kg]
Kf=1.86;//cryoscopic constant of water[K*Kg/mol]
```

```
dTf=0.16;//Lowering in freezing point[K]

//To find the molecular weight of sucrose
a=m1*dTf;
b=Kf*m2;
M2=b/a;//molecular weight
printf("M2=molecular weight ,    then M2=%f",M2);
```

Scilab code Exa 6.16 numerical

```
//example 5.16

clear;
clc;

//Given:
dTf=0.088;//Lowering in freezing point[K]
m2=0.45;//mass of sulphur[gm]
m1=0.09955;//mass of benzene[gm]
Kf=5.07;//cryoscopic constant for benzene[K*Kg/mol]

//To find the molecular formula of sulphur
a=m1*dTf;
b=Kf*m2;
M2=b/a;//molecular weight of sulphur
printf("The molecular weight of sulphur is %f",M2);
x=M2/32;//no. of sulphur atoms
printf("\n The molecular formula of sulphur is S%f",
   x);
```

Scilab code Exa 6.17 numerical

```
//example 6.17
```

```

clear;
clc;

//Given:
m2=1.35;//mass of a macromolecule[gm]
V=100;//volume of solution[cm^3]
R=82;//Universal gas constant[atm.cm^3.K^-1]
T=300;//Temperature[K]
II=9.9;//osmotic pressure of the solution[cm]
d=1;//density
p=1013250;//Atmospheric pressure
g=980.67;//gravitational field


//To find the molar mass of macromolecule
a=m2*R*T*p;
b=V*9.9*d*g;
M2=a/b;//molar mass of macromolecule
printf(" M2 = molar mass of macromolecule , therefore M2 = %f g.mol^-1",M2);
```

Scilab code Exa 6.18 numerical

```
//example 6.18

clear;
clc;

//Given:
R=82;//Universal gas constant[atm.ml.K^-1.mol^-1]
T=298;//Temperature[K]
V=250;//volume of water[ml]
m2=2.6;//mass of the protein
M2=85000;//molar mass of protein[g.mol^-1]
```

```


//To find the osmotic pressure of a solution
n2=m2/M2;//no. of moles of protein
II=(n2*R*T)/V;//Osmotic pressure of a solution[atm]
printf("The osmotic pressure is %f atm ",II);
```

Scilab code Exa 6.19 numerical

```
//example 6.19

clear;
clc;

//Given:
R=8.314;//Universal gas constant[J.K^-1.mol^-1]
Tb=373.15;//Boiling point temperature[K]
M1=0.018;// mass of water[kg]
Hvap=40.7;//Enthalpy of vaporization[KJ.mol^-1]

//To find the Ebullioscopic constant of water
a=R*0.001*Tb^2*M1;
b=Hvap;
Kb=a/b;//Ebullioscopic constant of water[K.Kg.mol^-1]
printf("The Ebullioscopic constant of water is %f K.Kg.mol-1",Kb);
```

Scilab code Exa 6.20 numerical

```
//example 6.20

clear;
```

```
clc;

disp("CaF2(s)<=>CaF2(aq)<=>Ca+2(aq) + 2F-(aq)");

//Given:
Ksp=4*10^-11;//Solubility product of sparingly
   soluble salt CaF2

//To find the value of activity coefficient
x=Ksp/4;
Cs=x^0.33;//Solubility
y=Cs^2;
Y=(x/y)^0.33;//activity coefficient
printf("The activity coefficient is %f ",Y);
```

Scilab code Exa 6.21 numerical

```
//example 6.21

clear;
clc;

//Given:
R=8.314;//Universal gas constant[J/K/mol]
T=298;//Temperature[K]
F=96500;//Faraday's constant
Eo=0.98;//Standard e.m.f of the cell[Volts]
E=1.16;//e.m.f of the cell[Volts]
m=0.01;

//To find the mean activity coefficient of ZnCl2
   solution
a=R*T;
b=2*F;
x=a/b;
```

```
Y=exp((Eo-E-(x*log(4*m*m*m)))/(3*x));//mean activity coefficient
printf(”The mean activity coefficient is %f”,Y);
```

Scilab code Exa 6.22 numerical

```
//example 6.22

clear;
clc;

//Given:
M1=0.01;//no. of moles of KCl
M2=0.005;//no. of moles of MgCl2
M3=0.002;//no. of moles of MgSO4
M=0.1;//mass of water[Kg]
z11=1;
z12=1;
z21=2;
z22=1;
z31=2;
z32=2;

//To find the ionic strength in a solution
m1=M1/M;//molality of KCL[m]
m2=M2/M;//molality of MgCl2[m]
m3=M3/M;//molality of MgSO4[m]

I=0.5*[(m1*z11^2+m1*z12^2+m2*z21^2+2*m2*z22^2+m3*z31^2+m3*z32^2)];//[mol/Kg]

printf(”The Ionic strength of a solution is %f mol/Kg”,I);
```

Scilab code Exa 6.23 numerical

```
//example 6.23

clear;
clc;

//Given:
T=298;//Temperature[K]
P=1;//pressure [atm]
m=0.02;//Ionic strength of HCl solution in CH3OH[mol
    /Kg]
E=32.6;//Di-electric constant
d=0.787;//Density[gm/cm3]

//To find the mean activity coefficient
I=0.5*(0.02*1*1+0.02*1*1);//Ionic strength of HCl
    solution[mol/Kg]
a=I*d;
b=(E^3)*(298^3);
x=(a/b)^0.5;
Y=10^(-1.825*1000000*1*1*x);//mean activity
    coefficient
printf("The mean activity coefficient is %f ",Y);
```

Chapter 7

Statistical Thermodynamics

Scilab code Exa 7.1 numerical

```
//example 7.1

clear;
clc;

//Given:
N=20;//no, of particles
N1=4;//no. of particles in E1 energy level
N2=4;//no. of particles in E2 energy level
N3=6;//no. of particles in E3 energy level
N4=3;//no. of particles in E4 energy level
N5=3;//no. of particles in E5 energy level
//To find the number of ways of distributing N
   particles
N!=prod(1:N);
N1!=prod(1:N1);
N2!=prod(1:N2);
N3!=prod(1:N3);
N4!=prod(1:N4);
N5!=prod(1:N5);
n=N1!*N2!*N3!*N4!*N5!;
```

```
W=N!/n;//no. of ways of distributing
disp(W,'The no. of ways of distributing the particles is ');
```

Scilab code Exa 7.2 numerical

```
//example 7.2

clear;
clc;

//Given:
T=298;//Temperature [K]
v=6.5*10^13;//Frequency in [sec-1]
//Consider zero point energy = 0.
h=6.627*10^-34;//planck's constant[J.s]
k=1.381*10^-23;//Boltzmann constant
N=1;//Since N=summation(gj*exp(-Ej/kT))

//To find the fraction of molecules present in vibrational level
E1=h*v;//for energy level 1[J]
E2=2*h*v;//for energy level 2[J]
x=k*T;
g1=1;
g2=1;
N1=[g1*exp(-E1/x)];//molecules present in energy level 1
N2=[g2*exp(-E2/x)];//molecules present in energy level 2
n1=N1/N;//fraction of molecules present in energy level 1
n2=N2/N;//fraction of molecules present in energy level 2
printf("The fraction of molecule s present in
```

```
energy level 1 is %f”,n1);


disp(n2,'The fraction of molecules present in energy level 2 is ');
```

Scilab code Exa 7.3 numerical

```
//example 7.3

clear;
clc;

//Given:
dE=4.3*10^-20;//difference in energy levels[J]
T1=0.000001;//Initial Temperature[K](approximately zero , needed for execution)
T2=300;//Final Temperature[K]
k=1.381*10^-23;//Boltzmann constant [J/K]

//To find the ratio of no. of particle per state for two states separated by an energy dE
x1=k*T1;
r1=exp(-dE/x1);
x2=k*T2;
r2=exp(-dE/x2);
disp(r1,'The ratio of no. of particles per state at 0K is ');
disp(r2,'The ratio of no. of particles per state at 300K is ');
```

Scilab code Exa 7.4 numerical

```
//example 7.4


clear;
clc;

//Given:
T1=273;//[K]
T2=14273;//[K]
E1=-13.6;//Energy of ground state [eV]
k=8.617*10^-5;//Boltzmann constant[eV/K]
g2=8;//total no. of states with energy E2
g1=2;//total no. of states with energy E1


//To find the no. of atoms in first-excited singlet
    state
E2=E1/(2^2);//Energy for n=2 (i.e.E2=E1/n2)
x1=k*T1;
r1=(g2/g1)*exp(-(E2-E1)/x1);
x2=k*T2;
r2=(g2/g1)*exp(-(E2-E1)/x2);
disp(r1,'The fraction of atoms present in level n=2
    at 273K is ');
disp("Therefore total 3*10^25 atoms we say   that
    all are present at ground     state");
printf("\n\nThe fraction of atoms present in level n
    =2 at 14273 is %f\n",r2);
x=r2*3*10^25;
disp(x,'Therefore no. of atoms in level n=2 is ');
```

Scilab code Exa 7.5 numerical

```
//example 7.5

```

```
clear;
clc;

//Given:
r1=0.001;//the population of the states at a higher energy to that at a lower energy
dE=8*10^-20;//The difference in energy[J]
k=1.381*10^-23;//Boltzmann constant [J/K]


//To find the Temperature at this condition
x=k*log(r1);
T=-dE/x;//[K]
printf("The Temperature at this condition is %f K",T);
```

Scilab code Exa 7.6 numerical

```
//example 7.6

clear;
clc;


//section(1)
//Given:
//The energy levels are not degenerate
w=1;//no. of ways of distributing the molecules
k=1.381*10^-23;//Boltzmann constant[J/K]
//To find the entropy of the system
S1=k*log(w);//Entropy of system at 0K
printf("The Entropy of System at 0K and non-degenerate eng level is %f J/K/mol",S1);

//section(2)
```

```
//Here the energy levels are degenerate
n=2;
R=8.314;//Universal gas constant[J/K/mol]

//To find the entropy of the system
//S=klog(n^N)=>S=R*log(n)
S2=R*log(n);//Entropy of the system[J/K/mol]
printf("\nThe Entropy of system at 0K and degenerete
    eng level is %f J/K/mol",S2);
```

Scilab code Exa 7.9 numerical

```
//example 7.9

clear;
clc;

//Given:
V=0.001;//Volume of vessel[m3]
T=300;//Temperature [K]
k=1.381*10^-23;//Boltzmann constant[J/K]
mol.wt=32;//molecular mass of oxygen molecule
h=6.626*10^-34;//planck's constant[J.s}



//To find the Transitional partition function of an
    oxygen molecule confined in a 1-litre vessel at
    300K
m=32*1.66*(10^-27);//mass of oxygen molecule[Kg]
x=[(2*3.14*m*k*T)^(3/2)]*V;
y=h^3;
zt=x/y;//Transitional partition function of an
    oxygen molecule
disp(zt,'The Transitional partition function of an
```

```
oxygen molecule confined in a 1-litre vessel at 300K is')
```

Scilab code Exa 7.12 numerical

```
//example 7.12

clear;
clc;

//Given:
R=1.99;//Universal gas constant [cal/K]
e=2.718;
V=22414;//volume[cm3]
L=6.023*10^23;
h=6.626*10^-27;//Planck's constant [erg.sec]
m=6.63*10^-23;//mass[gm]
k=1.381*10^-16;//Boltzmann constant[erg/K]
T=273.2;//Temperature[K]

//To find the Entropy of argon at 273K and 1 atmospheric pressure
x=V*(e^2.5);
y=L*(h^3);
z=(2*3.14*m*k*T)^1.5;
S=R*log(x*z/y);//Entropy [cal/degree/mol]
printf("The Entropy of argon at 273K and 1 atm is %f cal/degree/mol",S);
```

Scilab code Exa 7.14 numerical

```
//example 7.14

```

```
clear;
clc

//Given:
T=298;//Temperature[K]
I=1.9373*10^-46;//moment of inertia of O2 gas [Kg/m2]
h=6.626*10^-34;//Planck's constant[J.s]
k=1.381*10^-23;//Boltzmann constant[J/K]
R=8.314;//Universal gas constant[J/K/mol]
u=2;//Homonuclear diatomic molecule


//To find the rotational entropy and free energy for O2 gas
Sr=R+R*log(8*3.14*3.14*I*k*T/(u*h*h));//[J/K/mol]
Gr=-R*0.001*T*log(8*3.14*3.14*I*k*T/(u*h*h));//[KJ/mol]
printf("The rotational entropy for O2 gas is %f J/K/mol",Sr);
printf("\nThe rotational free energy for O2 gas is %f KJ/mol",Gr);
```

Scilab code Exa 7.15 numerical

```
//example 7.15

clear;
clc;

//Given:
T=298;//Temperature[K]
v=892.1*3*10^10;//frequency[sec-1]
h=6.626*10^-27;//Planck's constant [J.s]
k=1.381*10^-16;//Boltzmann constant[erg/K]
```

```
e=2.718;
R=1.998;//Universal gas constant[cal/K]
//To find the vibrational contribution to the entropy of F2 at 298K
x=h*v/(k*T);
a=R*x*e^-x/(1-e^-x);//a=E-Eo/T
b=R*log(1-e^-x);//b=G-Eo/T
S=a-b;//[cal/deg]
printf("The vibrational contribution to the entropy of F2 is %f cal/deg",S);
```

Scilab code Exa 7.16 numerical

```
//example 7.16

clear;
clc;

//Given:
T=1273;//Temperature[K]
h=6.26*10^-27;//Planck's constant[J.s]
k=1.381*10^-16;//Boltzmann constant[erg/K]
T=1000;//Temperature[degrees]
m=3.82*10^-23;//mass of Na [gm]
I=(1.91*10^-23)*(3.078*10^-8)^2;//moment of inertia[gm.cm2]
dE=0.73*1.602*10^-12;//[erg]
v=159.23*(3*10^10);//frequency [s-1]
R=82;//universal gas constant[cm3.atm/deg]
u=2;//symmetry number
L=6.023*10^23;//avogadro's number

//To find the equilibrium constant
p=((3.14*m*k*T)^1.5)/h/h/h;
s=R*u*h*h/L/8/3.14/3.14/I/k;
```

```
q=1-(exp(-h*v/k/T));
r=exp(-dE/k/T);
Kp=p*s*q*r;//Equilibrium constant
printf(”The equilibrium constant is %f”,Kp);
```

Scilab code Exa 7.17 numerical

```
//example 7.17

clear;
clc;

//Given:
T=298;//Temperature[K]
m1=32;
m2=36;
m3=34;
u1=8;
u2=9;
u3=16*18/34;
z1=0.99924;
z2=0.99951;
z3=0.99940;
h=6.26*10^-27;//Planck's constant[J.s]
c=3*10^10;//Speed of light[m/s]
k=1.38*10^-16;//Boltzman's constant[erg/K]
vo1=1535.8;//vibration frequency of 16O18O [cm-1]
vo2=1580.4;//vibration frequency of 16O2 [cm-1]
vo3=1490.0;//vibration frequency of 18O2 [cm-1]
dE=0.5*h*c*(2*vo1-vo2-vo3);//[erg]
r=dE/k/T;


//To find the equilibrium constant for isotopic exchange reaction
```

```
a=m3^3/m2^1.5/m1^1.5;
b=(u3^2)*4/u2/u1;
c=z3^2/z2/z1;
Kp=a*b*c*exp(-r);
printf("The value of equilibrium constant for
   isotopic exchange reaction is %f",Kp);
```