Scilab Textbook Companion for Chemistry by R. Chang[1]

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Book Description

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Scilab numbering policy used in this document and the relation to the above book.

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

AP Appendix to Example(Scilab Code that is an Appednix to a particular Example of the above book)

For example, Exa 3.51 means solved example 3.51 of this book. Sec 2.3 means a scilab code whose theory is explained in Section 2.3 of the book.

Contents

List of Scilab Codes

Chapter 1

Chemistry The Study of Change

Scilab code Exa 1.1 Computation of density from mass and volume

```
1  // Computation of density from mass and volume
2
3  clear;
4  clc;
5
6  printf("\t Example 1.1\n");
7
8  m=301;//mass of gold, g
9  v=15.6;// volume of gold, cm^3
10
11 d=m/v;//density of gold, g/cm^3
12
13 printf("\t the density of gold is : %4.1f g/cm^3\n",
       d);
14
15
16 //End
```

Scilab code Exa 1.2 Computation of mass from density and volume

```
1 // Computation of mass from density and volume
2
3 clear;
4 clc;
5
6 printf("\t Example 1.2\n");
7
8 d=13.6;//density of mercury, g/ml
9 v=5.50;// volume of mercury, ml
10
11 m=d*v;//mass of mercury, g
12
13 printf("\t the mass of mercury is : %4.1f g\n",m);
14
15
16 //End
```

Scilab code Exa 1.3 Conversion among temperature scales

```
1 // Conversion among temperature scales
2
3 clear;
4 clc;
5
6 printf("\t Example 1.3\n");
7
8 //for Solder
9
10 C=224;//melting point of solder, C
11 F=C*9/5+32;//melting point of solder, F
```

```
12
13 printf("\t the melting point of solder is : %4.0f F\
      n",F);
14
15
16 //for Helium
17
18 F=-452;//boiling point of helium, F
19 C=(F-32)*5/9;//boiling point of helium, C
20
21 printf("\t the boiling point of helium is : %4.0f C\
      n",C);
22
23
24 //for Mercury
25
26 C=-38.9;//meltiing point of mercury, C
27 K=C+273.15;//meltiing point of mercury, K
28
29 printf("\t the meltiing point of mercury is : %4.2f
      K\n",K);
30
31 //End
```

Scilab code Exa 1.5 Significant figures

```
1 // Significant figures
2
3 clear;
4 clc;
5
6 printf("\t Example 1.5\n");
7
8 //(a)
9 A=11254.1;//g
```

```
10 B=0.1983;//g
11 C=A+B;//g
12
13 printf("\t(a) ( %5.1f + %1.4f )g = %6.1f g\n",A,B,C)
      ;
14
15 //(b)
16 A=66.59;//L
17 B=3.113;//L
18 C=A-B;//L
19
20 printf("\t(b) ( %5.2f - %1.4f )L = %6.2f L\n",A,B,C)
      ;
21
22 //(c)
23 A=8.16;//m
24 B=5.1355;
25 C=A*B;//m
26
27 printf("\t(c) %5.2f m * %1.4f = %6.1f m\n",A,B,C);
28
29 //(d)
30 A=0.0154;//kg
31 B=88.3;//mL
32 C=A/B;//kg/mL
33
34 printf("\t(d) %1.4f kg / %2.1f mL = %1.2f *10^-4 kg/
      mL\n",A,B,C*10^4);
35
36 //(e)
37 A=2.64*10^3;//cm
38 B=3.27*10^2;//cm
39 C=A+B;//cm
40
41 printf("\t(e) ( %1.2f *10^3 + %1.2f *10^2 )cm = %1.2
      f *10^3 cm\n",A*10^-3,B*10^-2,C*10^-3);
42
43 //End
```

Scilab code Exa 1.6 Dimensional Analysis

```
1 // Dimensional Analysis
2
3 clear;
4 clc;
5
6 printf("\t Example 1.6\n");
7
8 lb=0.0833;//pound mass, lb
9
10 g=lb*453.6;//pound mass to gram mass, 1lb=453.6g
11
12 mg=1000*g;//gram to milligram
13
14 printf("\t the mass of glucose is : %1.2f *10^4 mg\n
   ",mg*10^-4);
15
16 //End
```

Scilab code Exa 1.7 Dimensional Analysis

```
1 // Dimensional Analysis
2
3 clear;
4 clc;
5
6 printf("\t Example 1.7\n");
7
8 L=5.2;//volume in litres
9
```

```
10 cc=1000*L;//litre to cm^3
11
12 mc=cc/10^6;//cm^3 to m^3
13
14 printf("\t the volume of blood is : %4.1f *10^-3 m
       ^3\n",mc*10^3);
15
16
17 //End
```

Scilab code Exa 1.8 Dimensional Analysis

```
1 // Dimensional Analysis
2
3 clear;
4 clc;
5
6 printf("\t Example 1.8\n");
7
8 gpcc=0.808;//density in gram per cm^3
9
10 kgpmc=1000*gpcc;//g/cm^3 to kg/m^3, as 1000g=1kg and
       1cm=10^-2 m
11
12 printf("\t the density of liquid nitrogen is : %3.0f
       kg/m^3\n",kgpmc);
13
14 //End
```

Chapter 3

Mass Relationships in Chemical Reactions

Scilab code Exa 3.1 Average Atomic Mass

```
1 // Average Atomic Mass
2
3 clear;
4 clc;
5
6 printf("\t Example 3.1\n");
7
8 Cu63=69.09;//percent of Cu 62.93 amu
9
10 Cu65=30.91;//percent of Cu 64.9278 amu
11
12 AverageAMU=62.93*Cu63/100+64.9278*Cu65/100;//
   average amu
13
14 printf("\t the average atomic mass of Copper is : %4
   .2f amu\n",AverageAMU);
15
16
17 //End
```

Scilab code Exa 3.2 Computation of number of moles from mass

```
1 // Computation of no. of moles from mass
2
3 clear;
4 clc;
5
6 printf("\t Example 3.2\n");
7
8 mass=6.46;//mass of He, g
9
10 moles=mass/4.003;//no. of moles of He, as mol. mass
   of He is 4.003 amu
11
12 printf("\t the no. of moles of He is : %4.2f mol\n",
   moles);
13
14
15 //End
```

Scilab code Exa 3.3 Computation of mass from moles

```
1 // Computation of mass from moles
2
3 clear;
4 clc;
5
6 printf("\t Example 3.3\n");
7
8 moles=0.356;//moles of Zn
9
```

```
10 mass=moles*65.39;//mass of Zn, g, 1 mole=65.39 g
11
12 printf("\t the mass of Zn is : %4.1f g\n",mass);
13
14
15 //End
```

Scilab code Exa 3.4 Computation of number of atoms from mass

```
1 // Computation of no. of atoms from mass
2
3 clear;
4 clc;
5
6 printf("\t Example 3.4\n");
7
8 Na=6.022*10^23;// Avogadro number, atoms/mol
9
10 mass=16.3;//mass of sulfur, g
11
12 moles=mass/32.07;//moles of S
13
14 atoms=moles*Na;//number of atoms of S
15
16 printf("\t the no. of atoms of S is : %4.2f*10^23\n"
   ,atoms*10^-23);
17
18
19 //End
```

Scilab code Exa 3.5 Computation of molecular mass of a compound

```
1 // Computation of molecular mass of a compound
```

```
2
3 clear;
4 clc;
5
6 printf("\t Example 3.5\n");
7
8 MassO=16;//mass of O, amu
9
10 //(a)
11 MassS=32.07;//mass of S, amu
12 MassSO2=MassS+MassO*2;//mass of SO2, amu
13
14 printf("\t the molecular mass of SO2 is : %4.2f amu\
   n",MassSO2);
15
16 //(b)
17 MassN=14.01;//mass of N, amu
18 MassH=1.008;//mass of H, amu
19 MassC=12.01;//mass of C, amu
20 MassC8H10N4O2=8*MassC+10*MassH+4*MassN+2*MassO;
21
22 printf("\t the molecular mass of C8H10N4O2 is : %4.2
   f amu\n",MassC8H10N4O2);
23
24 //End
```

Scilab code Exa 3.6 Computation of moles from mass of a compound

```
1 // Computation of moles from mass of a compound
2
3 clear;
4 clc;
5
6 printf("\t Example 3.6\n");
7
```

```
8  Mass=6.07;//mass of CH4, g
9  MassC=12.01;//mol. mass of C, amu
10 MassH=1.008;//mol. mass of H, amu
11 MassCH4=MassC+4*MassH;//mol. mass of CH4, amu
12
13 Moles=Mass/MassCH4;//no. of moles of CH4
14
15 printf("\t the no. of moles of CH4 is : %4.3f mol\n"
      ,Moles);
16
17 //End
```

Scilab code Exa 3.7 Computation of number of atoms from mass of a compound

```
1  // Computation of no. of atoms from mass of a
      compound
2
3  clear;
4  clc;
5
6  printf("\t Example 3.7\n");
7
8  Na=6.07*10^23;// Avogadro number, atoms/mol
9  Mass=25.6;//mass of Urea, g
10 MolMass=60.06;//mol. mass of Urea, g
11 moles=Mass/MolMass;//moles of Urea, mol
12 Atoms=moles*Na*4;//No. of atoms of Hydrogen
13
14 printf("\t the no. of atoms of hydrogen are : %4.2f
      *10^24 atoms\n",Atoms*10^-24);
15
16 //End
```

Scilab code Exa 3.8 Percentage composition of a compound

```
1 //Percentage composition of a compound
2
3 clear;
4 clc;
5
6 printf("\t Example 3.8\n");
7
8 H=1.008;//molar mass of H, g
9 P=30.97;//molar mass of P, g
10 O=16;//molar mass of O, g
11
12 MolMass=97.99;//mol. mass of H3PO4, g
13 percentH=3*H/MolMass*100;//percent of H
14 percentP=P/MolMass*100;//percent of P
15 percentO=4*O/MolMass*100;//percent of O
16
17 printf("\t the percent by mass of Hydrogen is : %4.3
   f percent\n",percentH);
18 printf("\t the percent by mass of Phosphorus is : %4
   .2f percent\n",percentP);
19 printf("\t the percent by mass of Oxygen is : %4.2f
   percent\n",percentO);
20
21 //End
```

Scilab code Exa 3.9 empirical formula of a compound from percentage composition

```
1 //empirical formula of a compound from percentage
   composition
```

```
2
3  clear;
4  clc;
5
6  printf("\t Example 3.9\n");
7
8  H=1.008;//molar mass of H, g
9  C=12.01;//molar mass of C, g
10 O=16;//molar mass of O, g
11
12 percentC=40.92;//percent of C
13 nC=percentC/C;
14
15 percentH=4.58;//percent of H
16 nH=percentH/H;
17
18 percentO=54.500;//percent of O
19 nO=percentO/O;
20
21 if(nC>nH) then// determining the smallest subscript
22     small=nH;
23 else small=nC;
24     if(small>nO) then
25         small=nO;
26     end
27 end;
28
29 nC=nC/small;//dividing by the smallest subscript
30 nH=nH/small;
31 nO=nO/small;
32 //the approximate values of these variables are to
     be multiplied by appropriate number to make it an
      integer by trial and error method
33 //in this case we need to multiply with 3 to get
     integer values
34 nC=nC*3;
35 nH=nH*3;
36 nO=nO*3;
```

```
37
38 printf("\t the empirical formula of ascorbic acid is
       : C%1.0f H%1.0f O%1.0f\n",nC,nH,nO);
39
40 //End
```

Scilab code Exa 3.10 mass of an element in a given compound

```
1 //mass of an element in a given compound
2
3 clear;
4 clc;
5
6 printf("\t Example 3.10\n");
7
8 massCuFeS2=3.71*10^3;//given mass of CuFeS2, kg
9 CuFeS2=183.5;//mol. mass of CuFeS2, g
10 Cu=63.55;//mol. mass of Cu, g
11 percentCu=Cu/CuFeS2*100;//percent Cu in CuFeS2
12 massCu=percentCu*massCuFeS2/100;//mass of Cu in
       given CuFeS2, kg
13
14 printf("\t the mass of Cu in CuFeS2 is : %1.2f*10^3
       kg\n",massCu*10^-3);
15
16 //End
```

Scilab code Exa 3.13 mass of an compound produced from certain mass of a given compound

```
1 //mass of an compound produced from certain mass of
       a given compound
2
```

```
3 clear;
4 clc;
5
6 printf("\t Example 3.13\n");
7
8 CO2=44.01;//mol. mass of CO2, g
9 Glucose=180.2;//mol. mass of Glucose, g
10 massGlucose=856;//given mass of Glucose, g
11 moleGlucose=massGlucose/Glucose;// moles of glucose
12 moleCO2=moleGlucose*6;//1 mole glucose gives 6 moles
       of CO2
13 massCO2=moleCO2*CO2;// mass of CO2, g
14
15 printf("\t the mass of CO2 is : %1.2f*10^3 g\n",
     massCO2*10^-3);
16
17 //End
```

Scilab code Exa 3.14 amount of reactants and products

```
1 //amount of reactants and products
2
3 clear;
4 clc;
5
6 printf("\t Example 3.14\n");
7
8 H2=2.016;//mol. mass of H2, g
9 Li=6.941;//mol. mass of Li, g
10 mH2=9.89;//mass of H2, g
11 nH2=mH2/H2;//moles of H2
12 nLi=2*nH2;//moles of Li, 1mol H2 given by 2mol Li
13 mLi=Li*nLi;////mass of Li, g
14
15 printf("\t the mass of Li is : %1.1f g\n",mLi);
```

```
16
17 //End
```

Scilab code Exa 3.15 limiting and excess reagent

```
1  //limiting and excess reagent
2
3  clear;
4  clc;
5
6  printf("\t Example 3.15\n");
7
8  Urea=60.06;//mol. mass of Urea, g
9  NH3=17.03;//mol. mass of NH3, g
10 CO2=44.01;//mol. mass of CO2, g
11
12 //(a)
13 //for NH3
14 mNH3=637.2;//mass of NH3, g
15 nNH3=mNH3/NH3;//moles of NH3
16 nUrea1=nNH3/2;//moles of Urea
17
18 //for CO2
19 mCO2=1142;//mol. mass of CO2, g
20 nCO2=mCO2/CO2;//moles of CO2
21 nUrea2=nCO2;//moles of Urea
22
23 if(nUrea1>nUrea2) then//finding limiting reagent
24     nUrea=nUrea2;
25     limiting="CO2";
26 else limiting="NH3";
27     nUrea=nUrea1;
28     end;
29 printf("\t the limiting reagent is : %s\n",limiting)
   ;
```

```
30
31 //(b)
32 mUrea=nUrea*Urea;//mass of urea produced
33 printf("\t the mass of the Urea produced is : %1.0f
      g\n",mUrea);
34
35 //(c)
36 if(limiting=="NH3") then//finding excess reagent
37     nCO2excess=nCO2-nNH3/2;
38     mCO2excess=nCO2excess*CO2;
39 printf("\t the mass of excess CO2 is : %1.0f g\n",
      mCO2excess);
40 else nNH3excess=nNH3-2*nCO2;
41      mNH3excess=nNH3excess*NH3;
42 printf("\t the mass of excess NH3 is : %1.0f g\n",
      mNH3excess);
43 end;
44
45 //End
```

Scilab code Exa 3.16 amount of reactants and products

```
1 //amount of reactants and products
2
3 clear;
4 clc;
5
6 printf("\t Example 3.16\n");
7
8 //(a)
9
10 //for TiCl4
11 mTiCl4=3.54*10^7;//mass of TiCl4, g
12 nTiCl4=mTiCl4/189.7;//moles of TiCl4
13 nTi1=nTiCl4*1;//moles of Ti
```

```
14
15 //for Mg
16 mMg=1.13*10^7;//mass of Mg, g
17 nMg=mMg/24.31;//moles of Mg
18 nTi2=nMg/2;//moles of Ti
19
20 if(nTi1>nTi2) then//finding imiting reagent
21       nTi=nTi2;
22 else nTi=nTi1;
23 end;
24 mTi=nTi*47.88;
25
26 printf("\t the theoretical yield is : %1.2f*10^6 g\n
     ",mTi*10^-6);
27
28 //(b)
29
30 mTiactual=7.91*10^6;//given, actual Ti produced
31 %yield=mTiactual/mTi*100;
32 printf("\t the percent yield is : %1.1f percent\n",
     %yield);
33
34 //End
```

Chapter 4

Reactions in aqueous solutions

Scilab code Exa 4.6 Computation of mass from concentration and volume

```
1 // Computation of mass from concentration and volume
2
3 clear;
4 clc;
5
6 printf("\t Example 4.6\n");
7
8 K2Cr2O7=294.2;//mol mass of K2Cr2O7, g
9
10 M=2.16;//Concentration of K2Cr2O7, M
11
12 V=0.250;//volume of K2Cr2O7, L
13
14 moles=M*V;//moles of K2Cr2O7
15
16 mass=moles*K2Cr2O7;
17
18 printf("\t the mass of the K2Cr2O7 needed is : %4.0f
     g\n",mass);
19
20 //End
```

Scilab code Exa 4.7 Computation of volume from concentration and mass

```
1 // Computation of volume from concentration and mass
2
3 clear;
4 clc;
5
6 printf("\t Example 4.7\n");
7
8 mGlucose=3.81;//mass of Glucose, g
9
10 Glucose=180.2;//mol mass of Glucose, g
11
12 M=2.53;//Concentration of Glucose, M
13
14 moles=mGlucose/Glucose;//moles of Glucose
15
16 V=moles/M;//volume of Glucose, L
17
18
19 printf("\t the volume of the Glucose needed is : %4
   .2f mL\n",V*1000);
20
21 //End
```

Scilab code Exa 4.8 Dilution of solution

```
1 // Dilution of solution
2
3 clear;
4 clc;
```

```
5
6  printf("\t Example 4.8\n");
7
8  M2=1.75;//final Concentration of H2SO4, M
9
10 V2=500;//final volume of H2SO4, mL
11
12 M1=8.61;//initial Concentration of H2SO4, M
13
14 V1=M2*V2/M1;//initail volume of H2SO4, mL
15
16 printf("\t the volume of the H2SO4 needed to dilute
      the solution is : %4.0f mL\n",V1);
17
18 //End
```

Scilab code Exa 4.9 Gravimetric Analysis

```
1  // Gravimetric Analysis
2
3  clear;
4  clc;
5
6  printf("\t Example 4.9\n");
7
8  mSample=0.5662;//mass of sample, g
9
10 Cl=35.5;//mol mass of Cl, g
11 AgCl=143.4;//mol mass of AgCl, g
12
13 mAgCl=1.0882;//mass of AgCl formed, g
14
15 %Cl(AgCl)=Cl/AgCl*100;//percent Cl in AgCl
16 mCl=%Cl(AgCl)*mAgCl/100;//mass of Cl in AgCl, g
17
```

```
18 //the same amount of Cl is present in initial sample
19
20 %Cl=mCl/mSample*100;//percent Cl in initial sample
21
22 printf("\t the percentage of Cl in sample is : %4.2f
       percent\n",%Cl);
23
24 //End
```

Scilab code Exa 4.10 Acid Base Titrations

```
1 // Acid Base Titrations
2
3 clear;
4 clc;
5
6 printf("\t Example 4.10\n");
7
8 mKHP=0.5468;//mass of KHP, g
9 KHP=204.2;//mol mass of KHP, g
10
11 nKHP=mKHP/KHP;//moles of KHP
12
13 VNaOH=23.48;//volume of NaOH, mL
14 MNaOH=nKHP/VNaOH*1000;//molarity of NaOH sol, M
15
16
17 printf("\t the molarity of NaOH solution is : %4.3f
     M\n",MNaOH);
18
19 //End
```

Scilab code Exa 4.11 Acid Base Titrations

```
// Acid Base Titrations

clear;
clc;

printf("\t Example 4.11\n");

MNaOH=0.610;//molarity of NaOH, M
VH2SO4=20;//volume of H2SO4, mL
MH2SO4=0.245;//molarity of H2SO4, M
nH2SO4=MH2SO4*VH2SO4/1000;//moles of H2SO4

VNaOH=2*nH2SO4/MNaOH;//Volume of NaOH, L

printf("\t the volume of NaOH solution is : %4.1f mL
   \n",VNaOH*1000);

//End
```

Scilab code Exa 4.12 Redox Titrations

```
// Redox Titrations

clear;
clc;

printf("\t Example 4.12\n");

MKMnO4=0.1327;//molarity of KMnO4, M
VKMnO4=16.42;//volume of KMnO4, mL
nKMnO4=MKMnO4*VKMnO4/1000;

nFeSO4=5*nKMnO4;
VFeSO4=25;//volume of FeSO4, mL

```

```
15 MFeSO4=nFeSO4/VFeSO4*1000;
16
17 printf("\t the molarity of FeSO4 solution is : %4.4f
       M\n",MFeSO4);
18
19 //End
```

Chapter 5

Gases

Scilab code Exa 5.1 Pressure Units

```
1 //Pressure Units
2
3 clear;
4 clc;
5
6 printf("\t Example 5.1\n");
7
8 Pbaro=688;//pressure in mm Hg
9 Patm=Pbaro/760;//pressure in atm
10
11 printf("\t the presuure in atmospheres is : %4.3f
     atm\n",Patm);
12
13 //End
```

Scilab code Exa 5.2 Pressure Units

```
1 //Pressure Units
```

```
2
3 clear;
4 clc;
5
6 printf("\t Example 5.2\n");
7
8 Pbaro=732;//pressure in mm Hg
9 Patm=Pbaro/760;//pressure in atm
10 P=Patm*1.01325*10^2;//pressure in kilo Pascal
11
12 printf("\t the presuure in kilo pascals is : %4.1f
     kPa\n",P);
13
14 //End
```

Scilab code Exa 5.3 Ideal Gas Equation

```
1 //Ideal Gas Equation
2
3 clear;
4 clc;
5
6 printf("\t Example 5.3\n");
7
8 V=5.43;//volume, L
9 t=69.5;//temperature, C
10 T=t+273;//temperature, K
11 n=1.82;//moles
12 R=0.0821;//universal gas constant, L.atm/(K.mol)
13 P=n*R*T/V;//pressure, atm
14
15 printf("\t the presuure in atmospheres is : %4.2f
     atm\n",P);
16
17 //End
```

Scilab code Exa 5.4 Ideal Gas Equation

```
1 //Ideal Gas Equation
2
3 clear;
4 clc;
5
6 printf("\t Example 5.4\n");
7
8 m=7.4;//mass of NH3, g
9
10 //at STP for NH3 for 1mole of NH3
11 V1=22.41;// volume, L
12 NH3=17.03;//molar mass of NH3, g
13
14 n=m/NH3;//moles of NH3
15 V=n*V1;//volume, L
16
17 printf("\t the volume of NH3 under given conditions
     is : %4.2f L\n",V);
18
19 //End
```

Scilab code Exa 5.5 Ideal Gas Equation

```
1 //Ideal Gas Equation
2
3 clear;
4 clc;
5
6 printf("\t Example 5.5\n");
```

```
7
8  V1=0.55;//volume, L
9  P1=1;//pressure at sea level, atm
10 P2=0.4;//pressurea at 6.5km height, atm
11
12 //n1=n2 and T1=T2 given hence P1V1=P2V2
13
14 V2=P1*V1/P2;
15
16 printf("\t the volume of He balloon at height 6.5km
       above sea level is : %4.1f L\n",V2);
17
18 //End
```

Scilab code Exa 5.6 Ideal Gas Equation

```
1  //Ideal Gas Equation
2
3  clear;
4  clc;
5
6  printf("\t Example 5.6\n");
7
8  P1=1.2;// pressure initial, atm
9  T1=18+273;//temperature initial, K
10 T2=85+273;//temperature final, K
11 //volume is constant
12
13 P2=P1*T2/T1;// pressure final,atm
14
15 printf("\t the final pressure is : %4.2f atm\n",P2);
16
17 //End
```

Scilab code Exa 5.7 Ideal Gas Equation

```
1 //Ideal Gas Equation
2
3 clear;
4 clc;
5
6 printf("\t Example 5.7\n");
7
8 P1=6.4;// pressure initial , atm
9 P2=1.0;// pressure final , atm
10 T1=8+273;//temperature initial , K
11 T2=25+273;//temperature final , K
12 V1=2.1;//volume initial , mL
13
14 V2=P1*V1*T2/(T1*P2);// volume final , mL
15
16 printf("\t the final volume is : %4.0f mL\n",V2);
17
18 //End
```

Scilab code Exa 5.8 Density Calulations

```
1 //Density Calulations
2
3 clear;
4 clc;
5
6 printf("\t Example 5.8\n");
7
8 //taking 1 mole of CO2
9 n=1;
```

```
10 R=0.0821;//universal gas constant, L. atm/K.mol
11 t=55;//temperature, C
12 T=t+273;//temperature, K
13 P=0.99;//.pressure, atm
14 M=44.01;//molar mass of CO2, g
15 d1=P*M/(R*T);//density of CO2, g/L
16
17 printf("\t the density of CO2 is : %4.2f g/L\n",d1);
18
19 //altenate method
20 //taking 1 mole of CO2
21 mass=M;//mass of CO2 in g =mol mass since we are
      considering 1 mole of CO2
22 V=n*R*T/P;//volume, L
23 d2=mass/V;//density=mass/volume, g/L
24
25
26 printf("\t (Alternate Method)the density of CO2 is :
       %4.2f g/L\n",d2);
27
28 //End
```

Scilab code Exa 5.9 Computation of Molar Mass of Gaseous substance

```
1 //Computation of Molar Mass of Gaseous substance
2
3 clear;
4 clc;
5
6 printf("\t Example 5.9\n");
7
8 d=7.71;// density, g/mL(given)
9 R=0.0821;//universal gas constant, L. atm/K.mol
10 T=36+273;// temp, K
11 P=2.88;//pressure, atm
```

```
12 M1=d*R*T/P;// mol. mass, g/mol
13 printf("\t the molecular mass of given compound is :
       %4.1f g/mol\n",M1);
14
15 //alternate method
16 //considering 1 L of compound
17 V=1;//volume, L
18 n=P*V/(R*T);//no of moles
19 m=7.71;//mass per 1 L, g
20 M2=m/n;// mol. mass, g/mol
21
22 printf("\t {alternate method} the molecular mass of
      given compound is : %4.1f g/mol\n",M2);
23 printf("\t the molecular formula can be only found
      by trial and error method as given in the book \n
      ");
24 //End
```

Scilab code Exa 5.10 Computation of Molar Mass

```
1 //Computation of Molar Mass
2
3 clear;
4 clc;
5
6 printf("\t Example 5.10\n");
7
8 percentSi=33;//percent of Si in compound
9 percentF=67;//percent of F in compound
10 nSi=percentSi/28.01;//moles of Si in 100g compound
11 nF=percentF/19;//moles of F in 100g compound
12
13 P=1.7;//pressure, atm
14 T=35+273;//temp. in K
15 m=2.38;//mass, g
```

```
16 V=0.21;//volume, L
17 R=0.0821;//universal Gas constant, L.atm/K.mol
18 n=P*V/(R*T);//moles
19 M=m/n;//mol. mass=mass/moles, g/mol
20
21 printf("\t the molecular mass of given compound is :
       %4.0f g/mol\n",M);
22
23
24 //End
```

Scilab code Exa 5.11 Gas Stoichiometry

```
1 //Gas Stoichiometry
2
3 clear;
4 clc;
5
6 printf("\t Example 5.11\n");
7
8 VC2H2=7.64;//volume of acetylene, L
9 VO2=VC2H2*5/2;//volume of O2 required for complete
     combustion as 5mol O2 react with 2mol acetylene
     for complete combustion
10
11 printf("\t the volume of O2 required for complete
     combustion of acetylene is : %4.1f L\n",VO2);
12
13
14 //End
```

Scilab code Exa 5.12 Gas Stoichiometry

```
1  //Gas Stoichiometry
2
3  clear;
4  clc;
5
6  printf("\t Example 5.12\n");
7
8  R=0.0821;//universal Gas constant, L.atm/K.mol
9  T=80+273;//temp in K
10 P=823/760;//pressure in atm
11 m=60;//mass of NaN3, g
12 NaN3=65.02;//mol. mass of NaN3, g
13 nN2=m*3/(2*NaN3);//moles of N2
14 VN2=nN2*R*T/P;//from ideal gas law
15
16 printf("\t the volume of N2 generated is : %4.1f L\n
     ",VN2);
17
18
19 //End
```

Scilab code Exa 5.13 Gas Stoichiometry

```
1  //Gas Stoichiometry
2
3  clear;
4  clc;
5
6  printf("\t Example 5.13\n");
7
8  R=0.0821;//universal Gas constant, L.atm/K.mol
9  T=312;//temp in K
10 V=2.4*10^5;//volume, L
11 P1=7.9*10^-3;//pressure initial in atm
12 P2=1.2*10^-4;//pressure final in atm
```

```
13 Pdrop=P1-P2;//pressure drop, atm
14 n=Pdrop*V/(R*T);//moles of Co2 reacted
15 Li2CO3=73.89;//mol. mass of Li2CO3, g
16 mLi2CO3=n*Li2CO3;//mass of Li2CO3, g
17
18 printf("\t the mass of Li2CO3 formed is : %4.1f
      *10^3 g\n",mLi2CO3*10^-3);
19
20
21 //End
```

Scilab code Exa 5.14 Daltons Law of Partial Pressures

```
1 //Dalton's Law of Partial Pressures
2
3 clear;
4 clc;
5
6 printf("\t Example 5.14\n");
7
8 nNe=4.46;//moles of Ne
9 nXe=2.15;//moles of Xe
10 nAr=0.74;//moles of Ar
11 PT=2;//total pressure in atm
12 XNe=nNe/(nNe+nAr+nXe);//mole fraction of Ne
13 XAr=nAr/(nNe+nAr+nXe);//mole fraction of Ar
14 XXe=nXe/(nNe+nAr+nXe);//mole fraction of Xe
15 PNe=XNe*PT;//partial pressure of Ne
16 PAr=XAr*PT;//partial pressure of Ar
17 PXe=XXe*PT;//partial pressure of Xe
18
19 printf("\t the partial pressures of Ne, Ar and Xe
      are : %4.2f atm, %4.2f atm and %4.3f atm
      respectively\n",PNe,PAr,PXe);
20
```

```
21
22 //End
```

Scilab code Exa 5.15 Daltons Law of Partial Pressures

```
1  //Dalton's Law of Partial Pressures
2
3  clear;
4  clc;
5
6  printf("\t Example 5.15\n");
7
8  PT=762;//pressure total, mmHg
9  PH2O=22.4;//pressure of water vapor, mmHg
10 PO2=PT-PH2O;//pressure of O2, frm Dalton's law, mmHg
11 M=32;//mol mass of O2, g
12 R=0.0821;//universal Gas constant, L.atm/K.mol
13 T=24+273;//temp in K
14 V=0.128;//volume in L
15 m=(PO2/760)*V*M/(R*T);//mass of mass of O2 collected
       , g
16
17 printf("\t the mass of O2 collected is : %4.3f g\n",
       m);
18
19
20 //End
```

Scilab code Exa 5.16 Root Mean Square velocity

```
1  //Root Mean Square velocity
2
3  clear;
```

```
4  clc;
5
6  printf("\t Example 5.16\n");
7
8  R=8.314;//universal Gas constant, J/K mol
9  T=25+273;//temp in K
10
11 //for O2
12 M=4.003*10^-3;//mol mass in kg
13 Urms=sqrt(3*R*T/M);//rms velocity, m/s
14
15 printf("\t the rms velocity of O2 collected is : %4
       .2f *10^3 m/s\n",Urms*10^-3);
16
17 //for N2
18 M=28.02*10^-3;//mol mass in kg
19 Urms=sqrt(3*R*T/M);//rms velocity, m/s
20
21 printf("\t the rms velocity of N2 collected is : %4
       .0f m/s\n",Urms);
22
23 //End
```

Scilab code Exa 5.17 Gas Effusion

```
1  //Gas Effusion
2
3  clear;
4  clc;
5
6  printf("\t Example 5.17\n");
7
8  t2=1.5;//diffusion time of compound, min
9  t1=4.73;//diffusion time of Br, min
10 M2=159.8;//mol mass of Br gas, g
```

```
11 M=(t2/t1)^2*M2;//molar gas of unknown gas, g(from
      Graham's Law of Diffusion)
12
13 printf("\t the molar mass of unknown gas is : %4.1f
      g/mol\n",M);
14
15 //End
```

Scilab code Exa 5.18 deviation from ideal behaviour

```
1 //deviation from ideal behaviour
2
3 clear;
4 clc;
5
6 printf("\t Example 5.18\n");
7
8 //(a)
9 V=5.2;//volume, L
10 T=47+273;
11 n=3.5;
12 R=0.0821;//universal Gas constant, L.atm/K.mol
13 P=n*R*T/V;
14
15 printf("\t the pressure of NH3 gas from ideal gas
      equation is : %4.1f atm\n",P);
16
17 //(b)
18 a=4.17;//constant, atm.L2/mol2
19 b=0.0371;//constant, L/mol
20 Pc=a*n^2/V^2;//pressure correction term, atm
21 Vc=n*b;//volume correction term, L
22 P=n*R*T/(V-Vc)-Pc;//from van der waals equation,
      pressure, atm
23
```

```
24 printf("\t the pressure of NH3 gas from van der
      waals equation is : %4.1f atm\n",P);
25
26 //End
```

Chapter 6

Thermochemistry

Scilab code Exa 6.1 work done by gas

```
1 //work done by gas
2
3 clear;
4 clc;
5
6 printf("\t Example 6.1\n");
7
8 //(a)
9 P=0;//external pressure, atm
10 Vf=6;//final volume, L
11 Vi=2;//initial volume, L
12 W=-P*(Vf-Vi);//work in atm.L
13
14 printf("\t the work done in expansion against vacuum
       is : %4.0f J\n",W);
15
16 //(b)
17 P=1.2;//external pressure, atm
18 Vf=6;//final volume, L
19 Vi=2;//initial volume, L
20 W=-P*(Vf-Vi);//work in atm.L
```

```
21 W=W*101.3;//work in J
22
23 printf("\t the work done in expansion against 1.2
      atm pressure is : %4.1f *10^2 J\n",W*10^-2);
24
25 //End
```

Scilab code Exa 6.2 change in energy of a gas

```
1 //change in energy of a gas
2
3 clear;
4 clc;
5
6 printf("\t Example 6.2\n");
7
8 q=-128;//heat transfer from the gas, J
9 w=462;//work done in compressing the gas, J
10 deltaE=q+w;//change in energy of the gas, J
11
12 printf("\t the change in energy for the process is :
      %4.0f J\n",deltaE);
13
14 //End
```

Scilab code Exa 6.3 heat produced in a reaction

```
1 //heat produced in a reaction
2
3 clear;
4 clc;
5
6 printf("\t Example 6.3\n");
```

```
7
8  mSO2=74.2;//mass in g
9  SO2=64.07;//molar mass in g
10 nSO2=mSO2/SO2;//moles of SO2
11 deltaH=-99.1;//heat produced for 1 mol, in kJ/mol
12 Hprod=deltaH*nSO2;//heat produced in this case, in
      kJ/mol
13
14 printf("\t the heat produced in a reaction is : %4.0
      f kJ\n",Hprod);
15
16 //End
```

Scilab code Exa 6.4 change in internal energy in a reaction

```
1  //change in internal energy in a reaction
2
3  clear;
4  clc;
5
6  printf("\t Example 6.4\n");
7
8  R=8.314;//gas constant, J/K. mol
9  T=298;//temp in K
10 deltaH=-566;//enthalpy change, kJ/mol
11 deltan=2-3;//change in gas moles
12 deltaE=deltaH-R*T*deltan/1000;//change in internal
      energy, kJ/mol
13
14 printf("\t the change in internal energy in the
      reaction is : %4.1f kJ/mol\n",deltaE);
15
16 //End
```

Scilab code Exa 6.5 amount of heat absorbed

```
1 //amount of heat absorbed
2
3 clear;
4 clc;
5
6 printf("\t Example 6.5\n");
7
8 m=466;//mass in g
9 s=4.184;//specific heat in J/g C
10 deltaT=74.6-8.5;//change in temp, C/K
11 q=m*s*deltaT;//amount of heat absorbed, kJ
12
13 printf("\t the amount of heat absorbed is : %4.0f kJ
   \n",q);
14
15 //End
```

Scilab code Exa 6.6 calculation of molar heat of combustion

```
1 //calculation of molar heat of combustion
2
3 clear;
4 clc;
5
6 printf("\t Example 6.6\n");
7
8 Ccal=10.17;//heat capacity, kJ/C
9 deltaT=25.95-20.28;//change in temp, C
10 qcal=Ccal*deltaT;
11 m=1.435;//mass of naphthalene, g
```

```
12 molm=128.2;//mol mass of naphthalene, g
13 q=-qcal*molm/m;//molar heat of combustion of
      naphthalene, kJ
14
15 printf("\t the molar heat of combustion of
      naphthalene is : %4.3f*10^3 kJ/mol\n",q*10^-3);
16
17 //End
```

Scilab code Exa 6.7 calculation of specific heat

```
1 //calculation of specific heat
2
3 clear;
4 clc;
5
6 printf("\t Example 6.7\n");
7
8 //for water
9 m=100;//mass, g
10 s=4.184;//specific heat, J/g C
11 deltaT=23.17-22.5;//change in temp., C
12 qH2O=m*s*deltaT;//heat gained by water, J
13
14 //for lead
15 qPb=-qH2O;//heat lost by lead, J
16 m=26.47;//mass, g
17 deltaT=23.17-89.98;//change in temp., C
18 s=qPb/(m*deltaT);//specific heat, J/g C
19
20 printf("\t the specific heat of lead is : %4.3f J/g
      C\n",s);
21
22 //End
```

Scilab code Exa 6.8 calculation of heat of neutralization

```
1 //calculation of heat of neutralization
2
3 clear;
4 clc;
5
6 printf("\t Example 6.8\n");
7
8 //for water
9 m=100+100;//mass, g
10 s=4.184;//specific heat, J/g C
11 deltaT=25.86-22.5;//change in temp., C
12 qsoln=m*s*deltaT/1000;//heat gained by water, kJ
13
14 qrxn=-qsoln;
15 Hneut=qrxn/(0.5*0.1);
16
17 printf("\t the heat of neutralization is : %4.1f kJ/
   mol\n",Hneut);
18
19 //End
```

Chapter 7

Quantum Theory and the Electronic Structure of Atoms

Scilab code Exa 7.1 calculation of speed of a wave

```
1 //calculation of speed of a wave
2
3 clear;
4 clc;
5
6 printf("\t Example 7.1\n");
7
8 lambda=17.4;//wavelength, cm
9 v=87.4;//frequency, Hz
10 u=lambda*v;//speed of wave, cm/s
11
12 printf("\t the speed of a wave is : %4.2f *10^3 cm/s
     \n",u*10^-3);
13
14 //End
```

Scilab code Exa 7.2 calculation of frequency of a wave

```
1 //calculation of frequency of a wave
2
3 clear;
4 clc;
5
6 printf("\t Example 7.2\n");
7
8 lambda=522*10^-9;//wavelength, m
9 c=3*10^8;//speed of light in vacuum, m/s
10 v=c/lambda;//frequency, Hz
11
12 printf("\t the frequency of the wave is : %4.2f
     *10^14 Hz\n",v*10^-14);
13
14 //End
```

Scilab code Exa 7.3 calculation of energy of a photon

```
1 //calculation of energy of a photon
2
3 clear;
4 clc;
5
6 printf("\t Example 7.3\n");
7
8 c=3*10^8;//speed of light in vacuum, m/s
9 h=6.63*10^-34;//planck's constant, J s
10 //(a)
11 lambda=5*10^-5;//wavelength, m
12 E=h*c/lambda;//energy, J
13
14 printf("\t (a) the energy of the photon is : %4.2f
     *10^-21 J\n",E*10^21);
```

```
15
16 //(b)
17 lambda=5*10^-11;//wavelength , m
18 E=h*c/lambda;//energy , J
19
20 printf("\t (b) the energy of the photon is : %4.2f
      *10^-15 J\n",E*10^15);
21
22 //End
```

Scilab code Exa 7.4 calculation of wavelength of a photon from an electronic transition

```
1 //calculation of wavelength of a photon from an
      electronic transition
2
3 clear;
4 clc;
5
6 printf("\t Example 7.4\n");
7
8 c=3*10^8;//speed of light in vacuum, m/s
9 h=6.63*10^-34;//planck's constant , J s
10 Rh=2.18*10^-18;//rydberg's constant , J
11 ni=5;//initial orbit
12 nf=2;//final orbit
13 deltaE=Rh*(1/ni^2-1/nf^2);
14 lambda=c*h/-deltaE;
15
16 printf("\t the wavelength of the photon is : %4.0f
      nm\n",lambda*10^9);
17
18 //End
```

Scilab code Exa 7.5 calculation of wavelength of a particle

```
1 //calculation of wavelength of a particle
2
3 clear;
4 clc;
5
6 printf("\t Example 7.5\n");
7
8 //(a)
9 h=6.63*10^-34;//planck's constant, J s
10 m=0.06;//mass, kg
11 u=63;//speed, m/s
12 lambda=h/(m*u);//wavelength, m
13
14 printf("\t the wavelength of the tennis ball is : %4
   .1f *10^-34 m\n",lambda*10^34);
15
16 //(b)
17 m=9.1094*10^-31;//mass, kg
18 u=68;//speed, m/s
19 lambda=h/(m*u);//wavelength, m
20
21 printf("\t the wavelength of the electron is : %4.1f
    *10^-5 m\n",lambda*10^5);
22
23 //End
```

Chapter 11

Intermolecular Forces and Liquids and Solids

Scilab code Exa 11.3 calculation of atomic radius

```
1 //calculation of atomic radius
2
3 clear;
4 clc;
5
6 printf("\t Example 11.3\n");
7
8 atoms=8*1/8+6*1/2;//atoms in a cell
9 d=19.3;//density, g/cc
10 Au=197;//mol mass of Au, g
11 NA=6.022*10^23;//avogadro no.
12 m=atoms*Au/NA;//mass of 1 cell, g
13 V=m/d;//volume, cc
14 a=V^(1/3);//edge length, cm
15 r=a/sqrt(8)/100;//radius in m
16
17 printf("\t the atomic radius of Au is : %4.0f pm\n",
     r*10^12);
18
```

```
19 //End
```

Scilab code Exa 11.4 diffraction

```
1 //diffraction
2
3 clear;
4 clc;
5
6 printf("\t Example 11.4\n");
7
8 n=1;
9 lambda=154;//wavelength , pm
10 theta=19.3;//angle of reflection , degree
11 d=n*lambda/(2*sin(theta*%pi/180));//spacing between
   the planes
12
13 printf("\t the spacing between planes is : %4.0f pm\
   n",d);
14
15 //End
```

Scilab code Exa 11.6 density of ionic crystals

```
1 //density of ionic crystals
2
3 clear;
4 clc;
5
6 printf("\t Example 11.6\n");
7
8 Na=22.99;//mass of one atom of Na, amu
9 Cl=35.45;//mass of one atom of Cl, amu
```

```
10 NA=6.022*10^23;//avogadro no.
11 mass=4*(Na+Cl)/NA;//mass in a unit cell in grams
12 a=564*10^-10;//edge length, cm
13 V=a^3;//volume of unit cell, cc
14 d=mass/V;//density in g/cc
15
16 printf("\t the density of NaCl is : %4.2f g/cc\n",d)
   ;
17
18 //End
```

Scilab code Exa 11.7 molar heat of vaporisation

```
1 //molar heat of vaporisation
2
3 clear;
4 clc;
5
6 printf("\t Example 11.7\n");
7
8 P1=401;//vapor pressure at 18C, mm Hg
9 T1=18+273;//temperature, K
10 T2=32+273;//temperature, K
11 deltaH=26000;//heat of vaporisation, J/mol
12 R=8.314;//gas constant, J/K.mol
13 X=deltaH/R*(T1-T2)/(T1*T2);
14 P2=401*exp(-X);//vapor pressure at 32C, mmHg(from ln
   (P1/P1)=deltaH/R*((T1-T2)/(T1*T2)))
15
16 printf("\t the pressure at 32 C is : %4.0f mm Hg\n",
   P2);
17
18 //End
```

Scilab code Exa 11.8 molar heat of vaporisation and overall energy required

```
1 //molar heat of vaporisation and overall energy
     required
2
3 clear;
4 clc;
5
6 printf("\t Example 11.8\n");
7
8 m=346;//mass of H2O in g
9
10 //from 0 to 100 C
11 s=4.184;//specific heat of H2O, J/g C
12 deltaT=100-0;//change in Temp, C
13 q1=m*s*deltaT/1000;//heating H2O, kJ
14
15 //for evaporation at 100 C
16 deltaH=40.79;//heat of vaporisation in kJ
17 H2O=18.02;//mol mass of H2O, g
18 q2=m*deltaH/H2O;//heat of vaporising water, kJ
19
20 //for steam from 100 to 182 C
21 deltaT=182-100;//change in temp of steam, kJ
22 s=1.99;//specific heat of steam, J/g C
23 q3=m*s*deltaT/1000;//heating steam, kJ
24
25 q=q1+q2+q3;//overall energy required, kJ
26
27 printf("\t the overall energy required is : %4.0f kJ
     \n",q);
28
29 //End
```

Chapter 12

Physical Properties of solutions

Scilab code Exa 12.2 computation of concentration of a solution

```
1 //computation of concentration of a solution
2
3 clear;
4 clc;
5
6 printf("\t Example 12.2\n");
7
8 msolute=0.892;//mass of solute, g
9 msolvent=54.6;//mass of solvent, g
10 percent=msolute/(msolute+msolvent)*100;//
   concentration, percent by mass
11
12 printf("\t the concentration of KCl solution is : %4
   .2f percent by mass\n",percent);
13
14 //End
```

Scilab code Exa 12.3 computation of molality of a solution

```
1 //computation of molality of a solution
2
3 clear;
4 clc;
5
6 printf("\t Example 12.3\n");
7
8 mass=24.4;//mass of H2SO4, g
9 M=98.09;//mol maass of H2SO4, g
10 n=mass/M;//moles of H2SO4
11 massH2O=0.198;//mass of H2O, kg
12 m=n/massH2O;//molality of H2SO4, molal
13
14 printf("\t the molality of sulfuric acid solution is
       : %4.2f m\n",m);
15
16 //End
```

Scilab code Exa 12.4 computation of molality from density and molarity

```
1 //computation of molality from density and molarity
2
3 clear;
4 clc;
5
6 printf("\t Example 12.4\n");
7
8 //considering 1L solution
9 msolution=976;//mass of solution, g
10 n=2.45;//moles
11 CH3OH=32.04;//mol. mass of CH3OH, g
12 msolute=n*CH3OH;//mass of solute, g
13 msolvent=(msolution-msolute)/1000;//mass of solvent,
       kg
14 m=n/msolvent;//molality, molal
```

```
15
16 printf("\t the molality of CH3OH solution is : %4.2f
       m\n",m);
17
18 //End
```

Scilab code Exa 12.5 computation of molality from mass percent

```
1 //computation of molality from mass percent
2
3 clear;
4 clc;
5
6 printf("\t Example 12.5\n");
7
8 //considering 100g of solution
9 percent=35.4;//mass percent of H3PO4
10 H3PO4=97.99;//mol mass of H3PO4
11 n=percent/H3PO4;//moles of H3PO4
12 mH2O=(100-percent)/1000;//mass of solvent
13 m=n/mH2O;//molality of H3PO4, molal
14
15 printf("\t the molality of H3PO4 solution is : %4.2f
       m\n",m);
16
17 //End
```

Scilab code Exa 12.6 computation of solubility of gases in liquid

```
1 //computation of solubility of gases in liquid
2
3 clear;
4 clc;
```

```
5
6 printf("\t Example 12.6\n");
7
8 c=6.8*10^-4;//solubility of N2 in water, M
9 P=1;//pressure, atm
10 k=c/P;//henry's constant
11
12 //for partial pressure of N2=0.78atm
13 P=0.78;//partial pressure of N2, atm
14 c=k*P;//solubility of N2, M
15
16 printf("\t the solubility of N2 gas in water is : %4
    .1f*10^-4 M\n",c*10^4);
17
18 //End
```

Scilab code Exa 12.7 computation of vapor pressure lowering

```
1 //computation of vapor pressure lowering
2
3 clear;
4 clc;
5
6 printf("\t Example 12.7\n");
7
8 H2O=18.02;//mol mass of H2O, g
9 V=460;//volume of water, mL
10 glucose=180.2;//mol. mass of glucose, g
11 mass=218;//mass of gllucose, g
12 n1=V/H2O;//moles of water
13 n2=mass/glucose;//moles of glucose
14 x1=n1/(n1+n2);//mole fraction of water
15 P=31.82;//vapor pressure of pure water, mmHg
16 P1=x1*P;//vapor pressure afteraddition of glucose,
    mmHg
```

```
17
18 printf("\t the vapor pressure lowering is : %4.1f
      mmHg\n",P-P1);
19
20 //End
```

Scilab code Exa 12.8 computation of freezing point depression and boiling point elevation

```
1  //computation of freezing point depression and
      boiling point elevation
2
3  clear;
4  clc;
5
6  printf("\t Example 12.8\n");
7
8  mH2O=2.505;//mass of H2O, kg
9  mEG=651;//mass of EG, g
10 EG=62.07;//mol mass of EG, g
11 n=mEG/EG;//moles of EG
12 m=n/mH2O;//molality of EG
13 Kf=1.86;//molal freezing point depression constant,
      C/m
14 deltaTf=Kf*m;//depression in freezing point, C
15 Kb=0.52;//molal boiling point elevation constant, C/
      m
16 deltaTb=Kb*m;//elevation in boiling point, C
17
18 printf("\t the depression in freezing point and
      elevation in boiling point are : %4.2f C and %4.1
      f C respectively\n",deltaTf,deltaTb);
19
20 //End
```

Scilab code Exa 12.9 computation of molar concentration from osmotic pressure

```
1 //computation of molar concentration from osmotic
     pressure
2
3 clear;
4 clc;
5 funcprot(0);
6
7 printf("\t Example 12.9\n");
8
9 pie=30;//osmotic pressure, atm
10 R=0.0821;//gas constant, L atm/K mol
11 T=298;//temp., K
12 M=pie/(R*T);//molar concentration, M
13
14 printf("\t the molar concentration is : %4.2f M\n",M
     );
15
16 //End
```

Scilab code Exa 12.10 computation of molar mass of a sample from freezing point depression

```
1 //computation of molar mass of a sample from
     freezing point depression
2
3 clear;
4 clc;
5
6 printf("\t Example 12.10\n");
```

```
7
8  deltaTf=1.05;//depression in freezing point, C
9  Kf=5.12;//molal freezing point depression constant
10 m=deltaTf/Kf;//molality of solution, molal
11 mbenzene=301/1000;//mass of benzene, kg
12 n=m*mbenzene;//moles of sapmle
13 msample=7.85;//mass of sample, g
14 molarmass=msample/n;//molar mass of sample, g/mol
15
16 printf("\t the molar mass of the sample is : %4.0f g
      /mol \n",molarmass);
17
18 //End
```

Scilab code Exa 12.11 computation of molar mass of a sample from osmotic pressure

```
1  //computation of molar mass of a sample from osmotic
       pressure
2
3  clear;
4  clc;
5  funcprot(0);
6
7  printf("\t Example 12.11\n");
8
9  R=0.0821;//gas constant, L atm/K mol
10 T=298;//temp, K
11 pie=10/760;//osmotic pressure, atm
12 M=pie/(R*T);//molarity of the solution, M
13
14 //taking 1L of solution
15 mass=35;//mass of Hg, g
16 n=M;//moles
17 molarmass=mass/n;//molar mass of hemoglobin, g/mol
```

```
18
19 printf("\t the molar mass of the hemoglobin is : %4
      .2f *10^4 g/mol \n",molarmass*10^-4);
20
21 //End
```

Scilab code Exa 12.12 computation of vant hoff factor

```
1 //computation of van't hoff factor
2
3 clear;
4 clc;
5 funcprot(0);
6
7 printf("\t Example 12.12\n");
8
9 R=0.0821;//gas constant, L atm/K mol
10 T=298;//temp, K
11 pie=0.465;//osmotic pressure, atm
12 M=0.01;//molarity of the solution, M
13 i=pie/(M*R*T);//vant hoff factor of KI
14
15 printf("\t the vant hoff factor of KI at 25 C is :
      %4.2f\n",i);
16
17 //End
```

Chapter 13

Chemical Kinetics

Scilab code Exa 13.2 computation of reaction rates using stoichiometry

```
1 //computation of reaction rates using stoichiometry
2
3 clear;
4 clc;
5
6 printf("\t Example 13.2\n");
7
8 dO2=-0.024;//rate of reaction of O2, M/s
9
10 //(a)
11 dN2O5=-2*dO2;//rate of formation of N2O5, M/s
12 printf("\t the rate of formation of N2O5 is : %4.3f
     M/s\n",dN2O5);
13
14 //(b)
15 dNO2=4*dO2;//rate of reaction of NO2, M/s
16 printf("\t the rate of reaction of NO2 is : %4.3f M/
     s\n",dNO2);
17
18 //End
```

Scilab code Exa 13.3 computation of reaction rates using initial rate data

```
1 //computation of reaction rates using initial rate
     data
2
3 clear;
4 clc;
5
6 printf("\t Example 13.3\n");
7
8 NO1=5*10^-3;//conc of NO from 1st experiment, M
9 H21=2*10^-3;//conc of H2 from 1st experiment, M
10 r1=1.3*10^-5;//initial rate from 1st experiment, M/s
11
12 NO2=10*10^-3;//conc of NO from 2nd experiment, M
13 H22=2*10^-3;//conc of H2 from 2nd experiment, M
14 r2=5*10^-5;//initial rate from 1st experiment, M/s
15
16 NO3=10*10^-3;//conc of NO from 3rd experiment, M
17 H23=4*10^-3;//conc of H2 from 3rd experiment, M
18 r3=10*10^-5;//initial rate from 3rd experiment, M/s
19
20 //(a)
21 //r=k*NO^x*H2^y, dividing r2/r1 and r3/r2
22 x=log(r2/r1)/log(NO2/NO1);//since H21=H22
23 y=log(r3/r2)/log(H23/H22);//since NO3=NO2
24 x=round(x);
25 y=round(y);
26
27 printf("\t (a) the rate of reaction is : r=k[NO]^%1
     .0f*[H2]^%1.0f\n",x,y);
28
29 //(b)
30 k=r2/((NO2)^x*H22^y);//rate constant, /M^2 s
```

```
31 printf("\t (b) the rate constant of the reaction is
      : %2.1f*10^2 /M^2 s\n",k*10^-2);
32
33 //(c)
34 NO=12*10^-3;//conc of NO, M
35 H2=6*10^-3;//conc of H2, M
36 rate=k*(NO^x)*H2^y;//rate , M/s
37 printf("\t (c) the rate of reaction at given
      concentration is : %1.1f*10^-4 M/s\n",rate*10^4);
38
39 //End
```

Scilab code Exa 13.4 calculations for first order reactions

```
1 //calculations for first order reactions
2
3 clear;
4 clc;
5
6 printf("\t Example 13.4\n");
7
8 t=8.8*60;//time , s
9 k=6.7*10^-4;//rate constant , s-1
10
11 //(a)
12 Ao=0.25;//initial conc , M
13 A=exp(-k*t+log(Ao));//final conc , M
14
15 printf("\t (a) the concentration of cyclopropane at
      given time is : %4.2f M\n",A);
16
17 //(b)
18 A=0.15;//initial conc , M
19 Ao=0.25;//final conc , M
20 t=-log(A/Ao)/(60*k);//time , min
```

```
21
22 printf("\t (b) the time required is : %2.0f min\n",t
   );
23
24 //(c)
25 percent=74;
26 //let initial conc be 1
27 Ao=1;//initial conc, M
28 A=1-percent/100;//final conc, M
29 t=-log(A/Ao)/(k*60);//time, min
30
31 printf("\t (c) the time required for required
   conversion is : %2.0f min\n",t);
32
33 //End
```

Scilab code Exa 13.5 calculation of rate constant from time and pressure data

```
1 //calculation of rate constant from time and
   pressure data
2
3 clear;
4 clc;
5
6 printf("\t Example 13.5\n");
7
8 t=[0,100,150,200,250,300];//time(data given), s
9 P=[284,220,193,170,150,132];//pressure(data given)
   in mmHg corresponding to time values
10 lnP=log(P);//lnP values corresponding to P
11
12 [slope]=reglin(t,lnP);//lnP=-k*t+lnPo, slope of the
   line between lnP and t gives -k value
13 k=-slope;//rate constant, s-1
```

```
14
15 printf("\t the rate constant for the decomposition
      is : %4.2f*10^-3 s-1\n",k*1000);
16
17 //End
```

Scilab code Exa 13.6 calculation of half life of first order reactions from rate constant

```
1 //calculation of half life of first order reactions
     from rate constant
2
3 clear;
4 clc;
5
6 printf("\t Example 13.6\n");
7
8 k=5.36*10^-4;//rate constant, s-1
9 t_half=0.693/(60*k);//half life of the reaction, min
10
11 printf("\t the half life for the decomposition of
     ethane is : %4.1f min\n",t_half);
12
13 //End
```

Scilab code Exa 13.7 calculation for second order reactions

```
1 //calculation for second order reactions
2
3 clear;
4 clc;
5
6 printf("\t Example 13.7\n");
```

```
7
8  k=7*10^9;//rate constant, M s
9
10 //(a)
11 t=2*60;//half life of the reaction, s
12 Ao=0.086;
13 A=(k*t+1/Ao)^-1;
14
15 printf("\t (a) the concentration of I is : %4.1f
      *10^-12 M\n",A*10^12);
16
17 //(b)
18 Ao=0.6;
19 t_half=1/(Ao*k);//half life of the reaction, s
20 printf("\t (b) the half life for Io=0.6 is : %2.1f
      *10^-10 s\n",t_half*10^10);
21
22 Ao=0.42;
23 t_half=1/(Ao*k);//half life of the reaction, s
24 printf("\t     the half life for Io=0.42 is : %2.1f
      *10^-10 s\n",t_half*10^10);
25
26 //End
```

Scilab code Exa 13.8 calculation of activation energy from rate constant and Temperature data

```
1 //calculation of activation energy from rate
     constant and Temperature data
2
3 clear;
4 clc;
5
6 printf("\t Example 13.8\n");
7
```

```
R=8.314;//gas constant, kJ/mol
T=[700,730,760,790,810];//temperature(data given), K
x=T^-1;//1/T values corresponding to Temp values above, K-1
k=[0.011,0.035,0.105,0.343,0.789];//rate constant(data given) in 1/M^1/2 s corresponding to temperature values
lnk=log(k);//lnk values corresponding to k
[slope]=reglin(x,lnk);//lnk=-Ea/(R*T)+lnA, slope of the line between lnk and 1/T gives -Ea/R value
Ea=-slope*R;//activation energy, kJ/mol

printf("\t the activation energy for the decomposition is : %4.2f*10^2 kJ/mol\n",Ea*10^-5);

//End
```

Scilab code Exa 13.9 calculation of rate constant at a given temperature

```
//calculation of rate constant at a given temperature

clear;
clc;

printf("\t Example 13.9\n");

k1=3.46*10^-2;//rate constant at T1
T1=298;//temp K
T2=350;//temp K
R=8.314;//gas constant,J/K mol
Ea=50.2*1000;//activation energy, J/mol
k2=k1/exp(Ea/R*(T1-T2)/(T1*T2));//from equation ln(k1/k2)=Ea*(T1-T2)/(T1*T2*R), S-1
```

```
14
15 printf("\t the rate constant at temp 350 is : %4.3f
      s-1\n",k2);
16
17 //End
```

Chapter 14

Chemical Equilibrium

Scilab code Exa 14.2 computation of equilibrium constant

```
1 //computation of equilibrium constant
2
3 clear;
4 clc;
5
6 printf("\t Example 14.2\n");
7
8 NO=0.0542;//equilibrium conc of NO, M
9 O2=0.127;//equilibrium conc of O2, M
10 NO2=15.5;//equilibrium conc of NO2, M
11
12 Kc=NO2^2/(O2*NO^2);//equilibrium constant for given
   reaction
13
14 printf("\t the value of the equilibrium constant of
   the reaction is : %4.2f *10^5\n",Kc*10^-5);
15
16 //End
```

Scilab code Exa 14.3 computation of component pressure from equilibrium constant

```
1 //computation of component pressure from equilibrium
      constant
2
3 clear;
4 clc;
5
6 printf("\t Example 14.3\n");
7
8 PCl3=0.463;//equilibrium pressure of PCl3, atm
9 PCl5=0.875;//equilibrium pressure of PCl5, atm
10 Kp=1.05;//equilibrium constant of the reaction
11
12 Cl2=Kp*PCl5/PCl3;//equilibrium pressure of Cl2 in
     atm, formula from the definition of equilibrium
     constant
13
14 printf("\t the value of the equilibrium pressure of
     the Cl2 gas is : %4.2f atm\n",Cl2);
15
16 //End
```

Scilab code Exa 14.4 computation of Kp from Kc

```
1 //computation of Kp from Kc
2
3 clear;
4 clc;
5
6 printf("\t Example 14.4\n");
7
8 Kc=10.5;
9 delta_n=1-3;
```

```
10 T=273+220;
11
12 Kp=Kc*(0.0821*T)^delta_n;
13
14 printf("\t the value of the equilibrium constant of
      the reaction is : %4.2f *10^-3\n",Kp*1000);
15
16 //End
```

Scilab code Exa 14.6 computation of Kp and Kc

```
1 //computation of Kp and Kc
2
3 clear;
4 clc;
5
6 printf("\t Example 14.6\n");
7
8
9 //(a)
10 CO2=0.236;//pressure of CO2 gas, atm
11 Kp=CO2;
12
13 //(b)
14 T=273+800;
15 delta_n=1;
16 Kc=Kp*(0.0821*T)^-delta_n;
17
18 printf("\t(a) the value of Kp of the reaction is :
      %4.3f\n",Kp);
19 printf("\t(b) the value of Kc of the reaction is :
      %4.2f *10^-3\n",Kc*1000);
20
21 //End
```

Scilab code Exa 14.8 Predicting the direction of a reaction

```
1 //Predicting the direction of a reaction
2
3 clear;
4 clc;
5
6 printf("\t Example 14.8\n");
7
8 Kc=1.2;//equilibrium constant for the reaction
9 N2=.249/3.5;//conc of N2, M
10 H2=(3.21*10^-2)/3.5;//conc of H2, M
11 NH3=(6.42*10^-4)/3.5;//conc of NH3, M
12
13 Qc=NH3^2/(N2*H2^3);//reaction quotient initial
14
15 if(Qc==Kc) then
16     d="the system is in equilibrium";
17 elseif(Qc<Kc) then
18     d="the system is not in equilibrium and the
       reaction will move from left to right";
19 else d="the system is not in equilibrium and the
   reaction will move from right to left";
20     end;
21
22 printf("\t %s\n",d);
23
24 //End
```

Scilab code Exa 14.9 computation of equilibrium concentration

```
1 //computation of equilibrium concentration
```

```
2
3 clear;
4 clc;
5
6 printf("\t Example 14.9\n");
7
8 Kc=54.3;
9 H2i=0.5;//initial moles of H2
10 I2i=0.5;//initial moles of I2
11
12 //Let us assume that x moles have reacted, so, HI=2x
    , H2=0.5-x, I2=0.5-x, when we substitute in Kc=(
    HI)^2/(H2)*(I2) we get 54.3=(2x)^2/((0.5-x)*(0.5-
    x)) taking root we get 7.37=2*x/0.5-x
13 x=0.393;//from the above equation
14 H2=0.5-x;
15 I2=0.5-x;
16 HI=2*x;
17
18 printf("\t the equilibrium concentration of H2 is :
    %4.3f M\n",H2);
19 printf("\t the equilibrium concentration of I2 is :
    %4.3f M\n",I2);
20 printf("\t the equilibrium concentration of HI is :
    %4.3f M\n",HI);
21
22 //End
```

Scilab code Exa 14.10 computation of equilibrium concentration

```
1 //computation of equilibrium concentration
2
3 clear;
4 clc;
5
```

```
6  printf("\t Example 14.10\n");
7
8  Kc=54.3;
9  HIo=0.0224;
10 H2o=0.00623;
11 I2o=0.00414;
12 //let us assume that x moles have reacted, so, HI=
      HIo+2x, H2=0.00623-x, I2=0.00414-x, when we
      substitute in Kc=(HI)^2/(H2)*(I2) we get 54.3=(2x
      +0.0224)^2/((0.00623-x)*(0.00414-x)) simplifying
      we get 50.3x^2-0.654x+8.98*10^-4=0
13 a=50.3;
14 b=-0.654;
15 c=8.98*10^-4;
16 x1=(-b+sqrt(b^2-4*a*c))/(2*a);
17 x2=(-b-sqrt(b^2-4*a*c))/(2*a);
18     if(x1>I2o)
19         x=x2;
20         else x=x1;
21     end;
22
23 H2=0.00623-x;
24 I2=0.00414-x;
25 HI=2*x+0.0224;
26
27 printf("\t the equilibrium concentration of H2 is :
      %4.5f M\n",H2);
28 printf("\t the equilibrium concentration of I2 is :
      %4.5f M\n",I2);
29 printf("\t the equilibrium concentration of HI is :
      %4.4f M\n",HI);
30
31 //End
```

Scilab code Exa 14.11 Application of Le chateliers Principle

```
1  //Application of Le chatelier's Principle
2
3  clear;
4  clc;
5
6  printf("\t Example 14.11\n");
7
8  //(b)
9  Kc=2.37*10^-3;//equilibrium constant for the
       reaction
10 N2=0.683;//conc of N2, M
11 H2=8.8;//conc of H2, M
12 NH3=3.65;//conc of NH3, M
13 Qc=NH3^2/(N2*H2^3);//reaction quotient initial
14
15 if(Qc==Kc) then
16     d="the system is in equilibrium";
17     elseif(Qc<Kc) then
18          d="the system is not in equilibrium and the
                reaction will move from left to right";
19         else d="the system is not in equilibrium and
               the reaction will move from right to
              left";
20     end;
21
22 printf("\t (b) %s\n",d);
23
24 //End
```

Chapter 15

Acids and Bases

Scilab code Exa 15.2 computation of hydronium ion concentration from hydroxide ion concentration

```
1 // computation of [H+] ion concentration from [OH-]
     ion concentration
2
3 clear;
4 clc;
5
6 printf("\t Example 15.2\n");
7
8 OH=0.0025 ;// [OH-] ion concentration, M
9 Kw=1*10^-14 ;// ionic product of water, M^2
10
11 H=Kw/OH; // From the formula (ionic product)Kw=[H
     +]*[OH-]
12 printf("\t The [H+] ion concentration of the
     solution is : %3.1f*10^-12 M\n",H*10^12);
13
14 //end
```

Scilab code Exa 15.3 Computation of pH of a solution from hydonium ion concentration

```
1 // Computation of pH of a solution from [H+] ion
     concentration
2
3 clear;
4 clc;
5
6 printf("\t Example 15.3\n");
7
8 H1=3.2*10^-4; //Concentration of [H+] ion on first
     occasion , M
9
10 pH1=-log10(H1);//from the definition of pH
11 printf("\t pH of the solution on first occasion is:
     %4.2f \n",pH1);
12
13 H2=1*10^-3; //Concentration of [H+] ion on second
     occasion , M
14
15 pH2=-log10(H2);//from the definition of pH
16 printf("\t pH of the solution on second occasion is
     : %4.2f \n",pH2);
17
18 //End
```

Scilab code Exa 15.4 Computation of hydronium ion concentration from pH

```
1 // Computation of [H+] ion concentration from pH
2
3 clear;
4 clc;
5
```

```
6 printf("\t Example 15.4\n");
7
8 pH=4.82;//Given
9 H=10^(-pH);//Concentration of [H+] ion, M, formula
    from the definition of pH
10
11 printf("\t The [H+] ion concentration of the
    solution is : %3.1f*10^-5 M\n",H*10^5);
12
13
14 //End
```

Scilab code Exa 15.5 Computation of pH of a solution from hydroxide ion concentration

```
1 // Computation of pH of a solution from [OH-] ion
    concentration
2
3 clear;
4 clc;
5
6 printf("\t Example 15.5\n");
7
8 OH=2.9*10^-4;//Concentration of [OH-] ion, M
9
10 pOH=-log10(OH);//by definition of p(OH)
11
12 pH=14-pOH;
13
14 printf("\t the pH of the solution is : %4.2f \n",pH)
    ;
15
16 //End
```

Scilab code Exa 15.6 Computation of pH of solutions for solutions of given concentrations

```
1 // Computation of pH of solutions for solutions of
     given concentrations
2
3 clear;
4 clc;
5
6 printf("\t Example 15.6\n");
7
8 //for HCL solution
9
10 ConcHCl=1*10^-3;//Concentration of HCl solution, M
11 H=ConcHCl;//Concentration of [H+] ion after
     ionisation of HCl
12 pH=-log10(H);
13 printf("\t the pH of the HCl solution is : %4.2f \n"
     ,pH);
14
15 //for Ba(OH)2 solution
16
17 ConcBaOH2=0.02;//Concentration of Ba(OH)2 solution,
     M
18 OH=ConcBaOH2*2;//Concentration of [OH-] ion after
     ionisation of Ba(OH)2 as two ions are generated
     per one molecule of Ba(OH)2
19 pOH=-log10(OH);
20 pH2=14-pOH;
21 printf("\t the pH of the Ba(OH)2 solution is : %4.2f
     \n",pH2);
22
23 //End
```

Scilab code Exa 15.8 Computation of pH for weak acid

```
1  // Computation of pH for weak acid
2
3  clear;
4  clc;
5
6  printf("\t Example 15.8\n");
7
8  InitHNO2=0.036;//Initial concentration of HNO2
       solution, M
9
10 //Let 'x' be the equilibrium concentration of the [H
       +] and [NO2-] ions, M
11
12 Ka=4.5*10^-4;//ionisation constant of HNO2, M
13 x=sqrt(Ka*InitHNO2);//from the definition of
       ionisation constant Ka=[H+]*[NO2-]/[HNO2]=x*x
       /(0.036-x), which reduces to x*x/0.036, as x<<
       InitHNO2 (approximation)
14
15 approx=x/InitHNO2*100;//this is the percentage of
       approximation taken. if it is more than 5%, we
       will be having higher deviation from correct
       value
16
17 if(approx>5)
18      x1=(-Ka+sqrt((Ka^2)-(-4*1*Ka*InitHNO2)))/(2*1);
19      x2=(-Ka-sqrt((Ka^2)-(-4*1*Ka*InitHNO2)))/(2*1);
20
21     if(x1>0)//as only one root is positive
22          x=x1;
23     else
24          x=x2;
```

```
25      end
26  end;
27
28  pH=-log10(x);//since x is the conc. of [H+] ions
29
30  printf("\t the pH of the HNO2 solution is : %4.2f \n
       ",pH);
31
32
33  //End
```

Scilab code Exa 15.9 Computation of ionisation constant from pH of a weak acid

```
1  // Computation of ionisation constant from pH of a
       weak acid
2
3  clear;
4  clc;
5
6  printf("\t Example 15.9\n");
7
8  pH=2.39;// pH of the HCOOH acid solution
9
10 InitHCOOH=0.1;//initial concentration of the
       solution
11 H=10^(-pH);//[H+] ion concentration from the
       definition of pH, M
12
13 Ka=(H^2)/(InitHCOOH-H);//ionisation constant of the
       acid , M, Ka=[H+]*[HCOO-]/[HCOOH]
14
15 printf("\t the ionisation constant of the given
       solution is : %4.2f*10^-4 M \n",10^4*Ka);
16
```

```
17 //End
```

Scilab code Exa 15.10 Computation of pH for weak base of given molarity

```
1  // Computation of pH for weak base of given molarity
2
3  clear;
4  clc;
5
6  printf("\t Example 15.10\n");
7
8  InitNH3=0.4;//Initial concentration of NH3 solution,
       M
9
10 //Let 'x' be the equilibrium concentration of the [
       OH-] and [NH4+] ions, M
11
12 Kb=1.8*10^-5;//ionisation constant of NH3, M
13 x=sqrt(Kb*InitNH3);//from the definition of
       ionisation constant Kb=[OH-]*[NH4+]/[NH3]=x*x/(
       InitNH3-x), which reduces to x*x/InitNH3, as x<<
       InitNH3 (approximation)
14
15 approx=x/InitNH3*100;//this is the percentage of
       approximation taken. if it is more than 5%, we
       will be having higher deviation from correct
       value
16
17 if(approx>5)
18      x1=(-Kb+sqrt((Kb^2)-(-4*1*Kb*InitNH3)))/(2*1);
19      x2=(-Kb-sqrt((Kb^2)-(-4*1*Kb*InitNH3)))/(2*1);
20
21     if(x1>0)//as only one root is positive
22          x=x1;
23     else
```

```
24            x=x2;
25        end
26    end;
27
28    pOH=-log10(x);//since x is the conc. of [H+] ions
29
30    pH=14-pOH;
31
32    printf("\t the pH of the NH3 solution is : %4.2f \n"
          ,pH);
33
34
35    //End
```

Scilab code Exa 15.11 Computation of concentration of all the species in solution of Oxalic acid

```
1  // Computation of concentration of all the species
       in solution of Oxalic acid
2
3  clear;
4  clc;
5
6  printf("\t Example 15.11\n");
7
8  InitC2H2O4=0.1;//Initial concentration of C2H2O4
       solution, M
9
10 //Let 'x1' be the equilibrium concentration of the [
       H+] and [C2HO4-] ions, M
11
12 //First stage of ionisation
13
14 Kw=10^-14;//ionic product of water, M^2
15 Ka1=6.5*10^-2;//ionisation constant of C2H2O4, M
```

```
16 x=sqrt(Ka1*InitC2H2O4);//from the definition of
     ionisation constant Ka1=[H+]*[C2HO4-]/[C2H2O4]=x*
     x/(InitC2H2O4-x), which reduces to x*x/InitC2H2O4
     , as x<<InitC2H2O4 (approximation)
17
18 approx=x/InitC2H2O4*100;//this is the percentage of
     approximation taken. if it is more than 5%, we
     will be having higher deviation from correct
     value
19
20 if(approx>5)
21       x1=(-Ka1+sqrt((Ka1^2)-(-4*1*Ka1*InitC2H2O4)))
           /(2*1);
22       x2=(-Ka1-sqrt((Ka1^2)-(-4*1*Ka1*InitC2H2O4)))
           /(2*1);
23
24      if(x1>0)//as only one root is positive
25           x=x1;
26      else
27           x=x2;
28      end
29 end;
30 C2H2O4=InitC2H2O4-x;//equilibrium value
31 printf("\t the concentration of the C2H2O4 in the
     solution is : %4.3f M\n",C2H2O4);
32
33
34 //Second stage of ionisation
35
36 InitC2HO4=x;//concentration of C2HO4 from first
     stage of ionisation
37
38 Ka2=6.1*10^-5;//ionisation constant of C2HO4-, M
39
40 //Let 'y' be the concentration of the [C2HO4-]
     dissociated to form [H+] and [C2HO4-] ions, M
41 y=Ka2;//from the definition of ionisation constant
     Ka2=[H+]*[C2O4-2]/[C2HO4-]=(0.054+y)*y/(0.054-y),
```

```
      which reduces to y, as y<<InitC2HO4 (
     approximation)
42
43 approx=y/InitC2HO4*100;//this is the percentage of
     approximation taken. if it is more than 5%, we
     will be having higher deviation from correct
     value
44
45 if(approx>5)
46       x1=(-Ka2+sqrt((Ka2^2)-(-4*1*Ka2*InitC2HO4)))
            /(2*1);
47       x2=(-Ka2-sqrt((Ka2^2)-(-4*1*Ka2*InitC2HO4)))
            /(2*1);
48
49      if(x1>0)//as only one root is positive
50           y=x1;
51      else
52           y=x2;
53      end
54 end;
55
56 C2HO4=InitC2HO4-y;//from first and second stages of
     ionisation
57 H=x+y;//from first and second stages of ionisation
58 C2O4=y;//from the assumption
59 OH=Kw/H;// From the formula (ionic product)Kw=[H+]*[
     OH-]
60
61 printf("\t the concentration of the [C2HO4-] ion in
     the solution is : %4.3f M\n",C2HO4);
62 printf("\t the concentration of the [H+] ion in the
     solution is : %4.3f M\n",H);
63 printf("\t the concentration of the [C2O4-2] ion in
     the solution is : %4.1f*10^-5 M\n",C2O4*10^5);
64 printf("\t the concentration of the [OH-] ion in the
      solution is : %f*10^-13 M\n",OH*10^13);
65
66
```

```
67 //End
```

Scilab code Exa 15.13 Computation of pH for a solution of salt of weak acid and strong base

```
1 // Computation of pH for a solution of salt of weak
     acid and strong base
2
3 clear;
4 clc;
5
6 printf("\t Example 15.13\n");
7
8 InitCH3COONa=0.15;//Initial concentration of
     CH3COONa solution , M
9
10 InitCH3COO=InitCH3COONa;//concentration of [CH3COO-]
     ion after dissociation of CH3COONa solution , M
11 //Let 'x' be the equilibrium concentration of the [
     OH-] and [CH3COOH] ions after hydrolysis of [
     CH3COO-], M
12
13 Kb=5.6*10^-10;//equilibrium constant of hydrolysis ,
     M
14
15 x=sqrt(Kb*InitCH3COO);//from the definition of
     ionisation constant Kb=[OH-]*[CH3COOH]/[CH3COO-]=
     x*x/(0.15-x), which reduces to x*x/0.15, as x
     <<0.15 (approximation)
16
17 approx=x/InitCH3COO*100;//this is the percentage of
     approximation taken. if it is more than 5%, we
     will be having higher deviation from correct
     value
18
```

```
19 if(approx>5)
20       x1=(-Kb+sqrt((Kb^2)-(-4*1*Kb*InitCH3COO)))
            /(2*1);
21       x2=(-Kb-sqrt((Kb^2)-(-4*1*Kb*InitCH3COO)))
            /(2*1);
22
23      if(x1>0)//as only one root is positive
24           x=x1;
25      else
26           x=x2;
27      end
28 end;
29
30 pOH=-log10(x);//since x is the conc. of [OH-] ions
31 pH=14-pOH;
32
33 printf("\t the pH of the salt solution is : %4.2f \n
      ",pH);
34
35 percenthydrolysis=x/InitCH3COO*100;
36 printf("\t the percentage of hydrolysis of the salt
      solution is : %5.4f percent\n",percenthydrolysis)
      ;
37
38 //End
```

Chapter 16

Acid Base Equilibria and Solubility Equilibria

Scilab code Exa 16.1 Computation of pH using common ion effect

```
1 // Computation of pH using common ion effect
2
3 clear;
4 clc;
5
6 printf("\t Example 16.1\n");
7
8 //(a)
9 InitCH3COOH=0.2;//Initial concentration of CH3COOH
     solution, M
10
11 //Let 'x' be the equilibrium concentration of the [H
     +] and [CH3COO-] ions after dissociation of [
     CH3COOH], M
12
13 Ka=1.8*10^-5;//equilibrium constant of acid, M
14
15 x=sqrt(Ka*InitCH3COOH);//from the definition of
     ionisation constant Ka=[H+]*[CH3COO-]/[CH3COOH]=x
```

```
    *x/(0.2-x), which reduces to x*x/0.2, as x<<0.2 (
    approximation)
16
17 pH=-log10(x);//since x is the conc. of [H+] ions
18
19 printf("\t (a) the pH of CH3COOH solution is : %4.2f
    \n",pH);
20
21 //(b)
22 InitCH3COONa=0.3;//Initial concentration of CH3COONa
    solution and is equal to conc of Na+ and CH3COO-
    as it completely dissociates, M
23
24 InitCH3COOH=0.2;//Initial concentration of CH3COOH
    solution, M
25 //Let 'x' be the equilibrium concentration of the [H
    +] and hence conc of [CH3COO-] ions is '0.3 + x',
    M
26
27 x=Ka*InitCH3COOH/InitCH3COONa;//from the definition
    of ionisation constant Ka=[H+]*[CH3COO-]/[CH3COOH
    ]=x*(0.3+x)/(0.2-x), which reduces to x*0.3/0.2(
    approximation)
28
29 pH=-log10(x);//since x is the conc. of [H+] ions
30
31 printf("\t (b) the pH of CH3COOH and CH3COONa
    solution is : %4.2f \n",pH);
32
33 //End
```

Scilab code Exa 16.3 Computation of pH using common ion effect

```
1 // Computation of pH using common ion effect
2
```

```
3 clear;
4 clc;
5
6 printf("\t Example 16.3\n");
7
8 Ka=1.8*10^-5;//ionisation constant of acid
9
10 //(a)
11 InitCH3COONa=1;//Initial concentration of CH3COONa
     solution and is equal to conc of Na+ and CH3COO-
     as it completely dissociates, M
12
13 InitCH3COOH=1;//Initial concentration of CH3COOH
     solution, M
14 //Let 'x' be the equilibrium concentration of the [H
     +] and hence conc of [CH3COO-] ions is '0.3 + x',
      M
15
16 x=Ka*InitCH3COOH/InitCH3COONa;//from the definition
     of ionisation constant Ka=[H+]*[CH3COO-]/[CH3COOH
     ]=x*(1+x)/(1-x), which reduces to x(approximation
     )
17
18 pH=-log10(x);//since x is the conc. of [H+] ions
19
20 printf("\t (a) the pH of CH3COOH and CH3COONa
     solution is : %4.2f \n",pH);
21
22 //(b)
23 HCl=0.1;//moles of HCl added to 1L solution
24 //as H+ reacts completely with CH3COO- ions to move
     the reaction forward
25 CH3COO=InitCH3COONa-HCl;//conc of CH3COO- ions, M
26 CH3COOH=InitCH3COOH+HCl;//conc of CH3COOH, M
27
28 //now for the equilibrium of CH3COOH and its ions,
     Let 'x' be the equilibrium concentration of the [
     H+] and hence conc of [CH3COO-] ions is 'CH3COO +
```

```
    x', M
x=Ka*CH3COOH/CH3COO;//from the definition of
    ionisation constant Ka=[H+]*[CH3COO-]/[CH3COOH]=x
    *(0.9+x)/(1.1-x), which reduces to x*0.9/1.1(
    approximation)

pH=-log10(x);//since x is the conc. of [H+] ions

printf("\t (b) the pH of solution after adding HCl
    is : %4.2f \n",pH);

//End
```

Scilab code Exa 16.5 Computation of pH in a titration of weak acid and strong base

```
// Computation of pH in a titration of weak acid and
    strong base

clear;
clc;

printf("\t Example 16.5\n");

InitCH3COOH=0.1;//Initial concentration of CH3COOH
    solution, M
VCH3COOH=25;//volumeof CH3COOH, mL
nCH3COOH=InitCH3COOH*VCH3COOH/1000;
Ka=1.8*10^-5;//equilibrium constant of acid, M
Kb=5.6*10^-10;//equilibrium constant of base, M

//(a)
N=0.1;//Initial concentration of NaOH solution, M
V=10;//Initial volume of NaOH solution, mL
n=N*V/1000;//Initial moles of NaOH solution
```

```
18
19 nCH3COOH_tit=nCH3COOH-n;//moles of CH3COOH after
      titration
20 nCH3COO=n;//moles of CH3COO after titration
21
22 H=nCH3COOH_tit*Ka/nCH3COO;//conc of H+ ions, M
23
24 pH=-log10(H);//since H is the conc. of [H+] ions
25
26 printf("\t (a) the pH of the solution is : %4.2f \n"
      ,pH);
27
28 //(b)
29 N=0.1;//Initial concentration of NaOH solution, M
30 V=25;//Initial volume of NaOH solution, mL
31 n=N*V/1000;//Initial moles of NaOH solution
32
33 nCH3COOH_tit=nCH3COOH-n;//moles of CH3COOH after
      titration
34 nCH3COO=n;//moles of CH3COO- ions after titration
35 V_total=V+VCH3COOH;//total volume after titration
36
37 CH3COO=nCH3COO/V_total*1000;//conc of CH3COO- ions,
     M
38 //Let 'x' be the equilibrium concentration of the [
      OH-] and [CH3COOH] ions after hydrolysis of [
      CH3COO-], M
39 x=sqrt(Kb*CH3COO);//from the definition of
      ionisation constant Kb=[OH-]*[CH3COOH]/[CH3COO-]=
      x*x/(0.05-x), which reduces to x*x/0.05, as x
      <<0.05 (approximation)
40
41 pOH=-log10(x);//since x is the conc. of [OH-] ions
42 pH=14-pOH;
43
44 printf("\t (b) the pH of the solution is : %4.2f \n"
      ,pH);
45
```

```
46 //(c)
47 N=0.1;//Initial concentration of NaOH solution, M
48 V=35;//Initial volume of NaOH solution, mL
49 n=N*V/1000;//Initial moles of NaOH solution
50
51 n_tit=n-nCH3COOH;//moles of NaOH after titration
52 nCH3COO=nCH3COOH;//moles of CH3COO- ions after
      titration
53 V_total=V+VCH3COOH;//total volume
54
55 OH=n_tit/V_total*1000;//conc of OH- ions, M
56 pOH=-log10(OH);//since OH is the conc. of [OH-] ions
57 pH=14-pOH;
58
59 printf("\t (c) the pH of the solution is : %4.2f \n"
      ,pH);
60
61 //End
```

Scilab code Exa 16.6 Computation of pH in a titration of weak base and strong acid at equivalence point

```
1 // Computation of pH in a titration of weak base and
      strong acid at equivalence point
2
3 clear;
4 clc;
5
6 printf("\t Example 16.6\n");
7
8 InitNH3=0.1;//Initial concentration of NH3 solution,
      M
9 VNH3=25;//volume of NH3, mL
10 nNH3=InitNH3*VNH3/1000;
11 Ka=5.6*10^-10;//equilibrium constant of acid, M
```

```
12
13 N=0.1;//Initial concentration, M
14 V=VNH3/InitNH3*N;//Initial volume, mL
15
16 V_total=V+VNH3;//total volume of the mixture, mL
17
18 n_NH4Cl=nNH3;//moles of NH4Cl
19 NH4Cl=n_NH4Cl/V_total*1000;//conc of NH4+ ions
     formed, M
20
21 //Let 'x' be the equilibrium concentration of the [H
     +] and [NH3] ions, M
22 x=sqrt(Ka*NH4Cl);//from the definition of ionisation
      constant Ka=[H+]*[NH3]/[NH4+]=x*x/(NH4+-x),
     which reduces to x*x/NH4+, as x<<NH4+ (
     approximation)
23
24 pH=-log10(x);//since x is the conc. of [H+] ions
25
26 printf("\t the pH of the solution at equivalent
     point is : %4.2f \n",pH);
27
28 //End
```

Scilab code Exa 16.8 Computation of Ksp from solubility

```
1 // Computation of Ksp from solubility
2
3 clear;
4 clc;
5
6 printf("\t Example 16.8\n");
7
8
9 //Let 's' be the equilibrium concentration of the [
```

```
   Ca2+] and [SO4 2-] ions, M
solubility=0.67;//solubility of CaSO4, g/L
M=136.2;//mol mass of CaSO4, g
s=solubility/M;//concentration, M
Ksp=s^2;//solubility product

printf("\t the Ksp of CaSO4 is : %2.1f*10^-5 \n",Ksp
   *10^5);

//End
```

Scilab code Exa 16.9 Computation of solubility from Ksp

```
// Computation of solubility from Ksp

clear;
clc;

printf("\t Example 16.9\n");

Ksp=2.2*10^-20;//solubility product
//Let 's' be the equilibrium concentration of the [
   Cu2+] and hence conc of [OH-] ions will be'2s', M
   , so Ksp=s*(2s)^2=4s^3

s=(Ksp/4)^(1/3);//concentration, M
M=97.57;//mol mass of Cu(OH)2, g
solubility=s*M;//solubility of Cu(OH)2, g/L

printf("\t the solubility of Cu(OH)2 is : %2.3f
   *10^-5 g/L\n",solubility*10^5);

//End
```

Scilab code Exa 16.10 Predicting precipitation reactions

```
1  // Predicting precipitation reactions
2
3  clear;
4  clc;
5
6  printf("\t Example 16.10\n");
7
8  Ksp=1.1*10^-10;//solubility product of BaSO4
9
10 //for Ba2+ ion
11 N=0.004;//normality , M
12 V=200;//vol in mL
13 n=N*V/1000;//moles
14
15 //for K2SO4sol
16 N1=0.008;//normality , M
17 V1=600;//vol in mL
18 n1=N1*V1/1000;//moles
19
20 Nnew=n*1000/(V+V1);//conc of Ba2+ ions in final sol
21 N1new=n1*1000/(V+V1);//conc of SO4 2- ions in final
      sol
22
23 Q=Nnew*N1new;//as Q=[Ba2+][SO4 2-]
24 if(Q>Ksp) then//determination of precipitation
25     printf("\t the solution is supersaturated and
         hence a precipitate will form\n");
26     else
27     printf("\t the solution is not supersaturated
         and hence a precipitate will not form\n");
28     end;
29 //End
```

Scilab code Exa 16.11 separation by fractional precipitation

```
1 //separation by fractional precipitation
2
3 clear;
4 clc;
5
6 printf("\t Example 16.11\n");
7
8 //for Br
9 Br=0.02;//conc of Ag+ ions, M
10 Ksp1=7.7*10^-13;//solubility product of AgBr
11 Ag1=Ksp1/Br;//conc of Ag+ ions at saturated state, M
12
13 //for Cl
14 Ksp2=1.6*10^-10;//solubility product of AgCl
15 Cl=0.02;//conc of Cl- ions, M
16 Ag2=Ksp2/Cl;//conc of Ag+ ions at saturated state, M
17
18 printf("\t to precipitate Br- without precipitating
   Cl- the concentration of Ag must be greater than
   %2.1f *10^-11 M but less than %2.1f *10^-9 M\n",
   Ag1*10^11,Ag2*10^9);
19
20 //End
```

Scilab code Exa 16.12 common ion effect and solubility

```
1 //common ion effect and solubility
2
3 clear;
4 clc;
```

```
5
6 printf("\t Example 16.12\n");
7
8 N_AgNO3=6.5*10^-3;//normality of AgNO3, M
9 AgCl=143.4;//mol mass of AgCl, g
10 //Let 's' be the molar solubility of AgCl in AgBr
   solution, M
11 Ksp=1.6*10^-10;//solubility product of AgCl
12 //Now Ag+ ion conc is AgNO3 conc + s and Cl- ion
   conc is 's', Now Ksp=[Ag+][Cl-]=(s+6.5*10^-3)*(s)
   =6.5*10^-3*s(approx as s<<6.5*10^-3)
13
14 Ag=N_AgNO3;//conc of Ag+ ions as 's' is negligible,
   M
15 s=Ksp/Ag;//as Ksp=[Ag+][Cl-], molar solubility of
   AgCl, M
16
17 solubility=s*AgCl;//solubility of AgCl in AgBr
   solution, g/L
18
19 printf("\t the solubility of AgCl in AgBr solution
   is : %2.2f *10^-6 g/L\n",solubility*10^6);
20
21 //End
```

Scilab code Exa 16.14 calculation of Concentration for precipitation

```
1 // calculation of Concentration for precipitation
2
3 clear;
4 clc;
5
6 printf("\t Example 16.14\n");
7
8 FeCl2=0.003;//normality of FeCl2, M
```

```
Fe=FeCl2;//as Fe2+ is strong electrolyte, conc of Fe2+=conc of FeCl2, M
Ksp=1.6*10^-14;//solubility product of FeCl2

OH=sqrt(Ksp/Fe);//as Ksp=[Fe2+][OH-]^2, conc of OH- ions, M

//Let 'x' be the initial concentration of the NH3, M
//conc of NH3 at equilibrium is 'x-OH' as NH3 hydrolyses to give OH- ions
Kb=1.8*10^-5;//ionisation constant of base

x=(OH^2)/Kb+OH;//as Kb=[NH4+][OH-]/[NH3]

printf("\t to initiate precipitation the conc of NH3 must be slightly greater than : %2.1f *10^-6 M\n",x*10^6);

//End
```

Scilab code Exa 16.15 Computation of concentration at complex ion equilibrium

```
//Computation of concentration at complex ion equilibrium

clear;
clc;

printf("\t Example 16.15\n");

CuSO4=0.2;//normality of CuSO4, M
NH3=1.2;//initial conc of NH3, M
VNH3=1;//volume of NH3, L
Kf=5*10^13;//formation constant
```

```
12 CuNH34=CuSO4;//conc of Cu(NH3)4 2+, M
13 NH3=NH3-4*CuNH34;//conc of NH3 after formation of
      complex, as 4 moles of NH3 react to form 1 mole
      complex, M
14
15 //let 'x' be the conc of Cu2+ ions
16 x=CuNH34/(NH3^4*Kf);//as Kf=[Cu(SO4)3 2+]/[Cu2+][NH3
      ]^4
17
18 printf("\t the conc of Cu2+ ions in equilibrium is :
       %2.1f *10^-13 M\n",x*10^13);
19
20 //End
```

Scilab code Exa 16.16 Computation of molar solubility in complex ion solution

```
1 //Computation of molar solubility in complex ion
     solution
2
3 clear;
4 clc;
5
6 printf("\t Example 16.16\n");
7
8 InitNH3=1;//initial conc of NH3, M
9 Ksp=1.6*10^-10;//solubility product of AgCl
10 Kf=1.5*10^7;//formation constant of complex
11 K=Ksp*Kf;//overall equilibrium constant
12
13 //let 's' be the molar solubility of AgCl, hence
     conc of [Ag(NH3)2+] and [Cl-] is 's' and hence
     conc of NH3 = InitNH3-2s
14 //K=[Ag(NH3)2+][Cl-]/[NH3]^2=s*s/(InitNH3-2s)^2,
     taking square root s/(InitNH3-2s)=sqrt(K)
```

```
15 s=sqrt(K)/(1+2*InitNH3*sqrt(K));//molar solubility
      of AgCl, M
16
17 printf("\t amount of AgCl which can be dissolved in
      1 L of 1 M NH3 sol in equilibrium is : %2.3f M\n"
      ,s);
18
19 //End
```

Chapter 17

Chemistry in the atmosphere

Scilab code Exa 17.1 computation of wavelength of a photon from energy

```
1 //computation of wavelength of a photon from energy
2
3 clear;
4 clc;
5
6 printf("\t Example 17.1\n");
7
8 E=498.7*10^3/(6.022*10^23);//energy in J/molecule
9 h=6.63*10^-34;//plancks constant, J s
10 v=E/h;//frequency of the photon, s^-1
11 lambda=3*10^8/v;//wavelength in m, since v*lambda=
   speed of light in vacuum
12
13 printf("\t the maximum wavelength of the photon
   which can dissociate an O2 molecule is : %4.0f nm
   \n",lambda*10^9);
14
15 //End
```

Scilab code Exa 17.3 Radioactive decay and half life

```
1 //Radioactive decay and half life
2
3 clear;
4 clc;
5
6 printf("\t Example 17.3\n");
7
8 Rninitial=1;//initial mass of Rn, g
9
10 Rnfinal=Rninitial*0.5^10;//final mass of Rn, g
11
12 printf("\t the amount of Rn left after 10 half lives
      is : %4.1f *10^-4 g\n",Rnfinal*10^4);
13
14 //End
```

Chapter 18

Entropy Free Energy and Equilibrium

Scilab code Exa 18.2 Entropy changes in the system

```
1 //Entropy changes in the system
2
3 clear;
4 clc;
5
6 printf("\t Example 18.2\n");
7
8 //(a)
9 SCaO=39.8;//standard entropy of CaO, J/K mol
10 SCO2=213.6;//standard entropy of CO2, J/K mol
11 SCaCO3=92.9;//standard entropy of CaCO3, J/K mol
12
13 deltaSrxn=SCaO+SCO2-SCaCO3;//standard entropy change
       of the reaction, J/K mol
14 printf("\t (a) the standard entropy of reaction is :
       %4.1f J/K mol\n",deltaSrxn);
15
16 //(b)
17 SNH3=193;//standard entropy of NH3, J/K mol
```

```
18 SN2=192;//standard entropy of N2, J/K mol
19 SH2=131;//standard entropy of H2, J/K mol
20
21 deltaSrxn=2*SNH3-(SN2+3*SH2);//standard entropy
      change of the reaction, J/K mol
22 printf("\t (b) the standard entropy of reaction is :
      %4.0f J/K mol\n",deltaSrxn);
23
24 //(c)
25 SHCl=187;//standard entropy of HCl, J/K mol
26 SH2=131;//standard entropy of H2, J/K mol
27 SCl2=223;//standard entropy of Cl2, J/K mol
28
29 deltaSrxn=2*SHCl-SH2-SCl2;//standard entropy change
      of the reaction, J/K mol
30 printf("\t (c) the standard entropy of reaction is :
      %4.0f J/K mol\n",deltaSrxn);
31 //End
```

Scilab code Exa 18.4 free energy changes in the system

```
1 //free energy changes in the system
2
3 clear;
4 clc;
5
6 printf("\t Example 18.4\n");
7
8 //(a)
9 GCO2=-394.4;//free energy of formation of CO2, kJ/
      mol
10 GH2O=-237.2;//free energy of formation of H2O, kJ/
      mol
11 GCH4=-50.8;//free energy of formation of CH4, kJ/mol
12 GO2=0;//free energy of formation of O2, kJ/mol
```

```
13
14 deltaGrxn=(GCO2+GH2O*2)-(GCH4+2*GO2);//standard free
       energy change of the reaction, kJ/mol
15
16 printf("\t (a) the standard free energy change of
       reaction is : %4.1f kJ/mol\n",deltaGrxn);
17
18 //(b)
19 GMg=0;//free energy of formation of Mg, kJ/mol
20 GMgO=-569.6;//free energy of formation of MgO, kJ/
       mol
21 GO2=0;//free energy of formation of O2, kJ/mol
22
23 deltaGrxn=(GO2+GMg*2)-(2*GMgO);//standard free
       energy change of the reaction, kJ/mol
24
25 printf("\t (b) the standard free energy change of
       reaction is : %4.0f kJ/mol\n",deltaGrxn);
26
27 //End
```

Scilab code Exa 18.5 entropy changes in the system for phase transitions

```
1 //entropy changes in the system for phase
      transitions
2
3 clear;
4 clc;
5
6 printf("\t Example 18.5\n");
7
8 //for fusion
9 T=5.5+273;//temperature of fusion, K
10 deltaH=10.9*1000;//change in enthalpy, J/mol
11 deltaSf=deltaH/T;//since in fusion deltaG=0, J/ K
```

```
    mol
12
13 //for vaporisation
14 T=80.1+273;//temperature of vaporisation, K
15 deltaH=31*1000;//change in enthalpy, J/mol
16 deltaSv=deltaH/T;//since in vaporisation deltaG=0, J
    / K mol
17
18 printf("\t the entropy change for fusion and
    condensation are : %4.1f J/K mol and %4.1f J/K
    mol respectively\n",deltaSf,deltaSv);
19
20 //End
```

Scilab code Exa 18.6 computation of equilibrium constant from free energy of a rxn

```
1 //computation of equilibrium constant from free
    energy of a rxn
2
3 clear;
4 clc;
5
6 printf("\t Example 18.6\n");
7
8 T=298;//temperature, K
9 R=8.314;//gas constant, J/K mol
10 GH2=0;//free energy of formation of H2, kJ/mol
11 GH2O=-237.2;//free energy of formation of H2O, kJ/
    mol
12 GO2=0;//free energy of formation of O2, kJ/mol
13 deltaG=1000*(2*GH2+GO2-2*GH2O);//free energy of rxn,
    J/mol
14
15 Kp=exp(-deltaG/(R*T));//equilibrium constant for rxn
```

```
16
17 printf("\t the equilibrium constant for the given
      reaction is : %2.0f*10^-84\n",Kp*10^84);
18
19 //End
```

Scilab code Exa 18.7 computation of free energy of a rxn from equilibrium constant

```
1 //computation of free energy of a rxn from
      equilibrium constant
2
3 clear;
4 clc;
5
6 printf("\t Example 18.7\n");
7
8 T=298;//temperature, K
9 R=8.314;//gas constant, J/K mol
10 Ksp=1.6*10^-10;//solubility constant
11 deltaG=-R*T*log(Ksp);//here solubility product is
      equal to equilibrium constant
12
13 printf("\t the free energy for the given reaction is
      : %4.0f kJ/mol \n",deltaG*10^-3);
14
15 //End
```

Scilab code Exa 18.8 computation of free energy of a rxn from conc of components

```
1 //computation of free energy of a rxn from conc of
      components
```

```
2
3  clear;
4  clc;
5
6  printf("\t Example 18.8\n");
7
8  T=298;//temperature, K
9  R=8.314;//gas constant, J/K mol
10 deltaG0=5.4*10^3;//standard free energy, kJ/mol
11 pNO2=0.122;//pressure of NO2, atm
12 pN2O4=0.453;//pressure of N2O4, atm
13 deltaG=deltaG0+R*T*log(pNO2^2/pN2O4);//here
      solubility product is equal to equilibrium
      constant
14
15 if(deltaG<0) then//equilibrium determination
16     d="net reaction proceeds from left to right to
          reach equilibrium";
17 else
18     d="net reaction proceeds from right to left to
          reach equilibrium";
19 end;
20 printf("\t the free energy for the given reaction is
      : %4.2f kJ/mol and %s\n",deltaG*10^-3,d);
21
22 //End
```

Chapter 19

Electrochemistry

Scilab code Exa 19.3 computation of standard emf of a cell

```
1 //computation of standard emf of a cell
2
3 clear;
4 clc;
5
6 printf("\t Example 19.3\n");
7
8 E0cathode=0.8;//standard electrode potential of
    cathode(Ag+/Ag), V
9 E0anode=-2.37;//standard electrode potential of
    anode(Mg2+/Mg), V
10
11 E0cell=E0cathode-E0anode;//standard emf of the cell,
    V
12
13 printf("\t the standard emf of the cell is : %4.2f V
    \n",E0cell);
14
15 //End
```

Scilab code Exa 19.4 computation of equilibrium constant for a reaction

```
1 //computation of equilibrium constant for a reaction
2
3 clear;
4 clc;
5
6 printf("\t Example 19.4\n");
7
8 n=2;
9 E0cathode=0.15;//standard electrode potential of
    cathode(Cu2+/Cu+), V
10 E0anode=-0.14;//standard electrode potential of
    anode(Sn2+/Sn), V
11
12 E0cell=E0cathode-E0anode;//standard emf of the cell,
    V
13
14 K=exp(n*E0cell/0.0257);//equilibrium constant, from
    the formula E0cell=0.0257*lnK/n
15
16 printf("\t the equilibrium constant for the given
    reaction is : %4.2f*10^9\n",K*10^-9);
17
18 //End
```

Scilab code Exa 19.5 computation of standard free energy change for a reaction

```
1 //computation of standard free energy change for a
    reaction
2
```

```
clear;
clc;

printf("\t Example 19.5\n");

n=6;
F=96500;//faraday constant, J/V mol

E0cathode=-2.87;//standard electrode potential of cathode(Ca2+/Ca), V
E0anode=1.5;//standard electrode potential of anode(Au3+/Au), V

E0cell=E0cathode-E0anode;//standard emf of the cell, V

deltaG0=-n*F*E0cell;//standard free energy change for the reaction, kJ/mol

printf("\t the standard free energy change for the reaction is : %4.2f*10^3 kJ/mol \n",deltaG0*10^-6);

//End
```

Scilab code Exa 19.6 computation of standard free energy change for a reaction

```
//computation of standard free energy change for a reaction

clear;
clc;

printf("\t Example 19.6\n");
```

```
7
8 n=2;
9 F=96500;//faraday constant, J/V mol
10
11 Co2=0.15;//conc of Co2+ ions, M
12 Fe2=0.68;//conc of Fe2+ ions, M
13
14 E0cathode=-0.44;//standard electrode potential of
     cathode(Fe2+/Fe), V
15 E0anode=-0.28;//standard electrode potential of
     anode(Co2+/Co), V
16
17 E0cell=E0cathode-E0anode;//standard emf of the cell,
     V
18
19 Ecell=E0cell-0.0257/2*log(Co2/Fe2);//calculation of
     cell potential at non standard conditions, V
20
21 if(Ecell>0) then
22     printf("\t the reaction would proceed
         spontaneously in the direction written \n");
23 else
24     printf("\t the reaction is not spontaneously in
         the direction written \n");
25     end;
26
27 //End
```

Scilab code Exa 19.7 computation of concentration of component from cell potential

```
1 //computation of concentration of component from
     cell potential
2
3 clear;
```

```
clc;

printf("\t Example 19.7\n");

n=2;

Zn=1;//conc of Zn2+ ions, M
pH2=1;//pressure of H2 gas, atm

Ecell=0.54;//emf of the cell, V

E0cell=0.76;//standard emf of the cell, V

Q=exp(-(Ecell-E0cell)*2/0.0257);//since Ecell=E0cell
   -0.0257/2*log(Q) where Q=(Zn2+)*pH2/(H+)^2

H=sqrt(Zn*pH2/Q);//the conc of H+ ions, M

printf("\t the molar concentration of H+ ion is : %2
   .0f*10^-4 M \n",H*10^4);

//End
```

Scilab code Exa 19.9 quantitative aspects of electrolysis

```
//quantitative aspects of electrolysis

clear;
clc;

printf("\t Example 19.9\n");

t=7.44*3600;//time, sec
A=1.26;//current in ampere
q=A*t;//charge passed, coulomb
```

```
11 F=96500;//faraday constant, J/V mol
12 ne=q/F;//moles of electrons
13 nO2=ne/4;//moles of oxygen
14 nH2=ne/2;//moles of H2
15
16 R=0.0821;//gas constant, L atm/K
17 T=273;//temperature in Kelvin
18 P=1;//pressure in atm
19 VO2=nO2*R*T/P;//volume of oxygen gas generated
20 VH2=nH2*R*T/P;//volume of H2 gas generated
21
22 printf("\t the volume of O2 gas and H2 gas generated
       are : %4.2f L and %4.2f L respectively\n",VO2,
     VH2);
23
24 //End
```

Chapter 23

Nuclear Chemistry

Scilab code Exa 23.2 calculation of nuclear binding energy

```
1 //calculation of nuclear binding energy
2
3 clear;
4 clc;
5
6 printf("\t Example 23.2\n");
7
8 NA=6.022*10^23;//avogadro number
9 c=3*10^8;//speed of light, m/s
10 p=1.007825;//mass of proton, amu
11 n=1.008665;//mass of neutron, amu
12 mI=126.9004;//atomic mass of I, amu
13 pI=53*p+74*n;//estimated mass of I, amu
14 deltam=mI-pI;//mass defect, amu
15 deltaE=-deltam*c^2;//energy released, amu m^2/s^2
16 deltaE=deltaE/(NA*1000);//energy released in J
17 deltaE=deltaE/127;//binding energy per nucleon, J
18
19 printf("\t the nuclear binding energy per nucleon is
    : %4.2f *10^-12 J/nucleon\n",deltaE*10^12);
20
```

```
21 //End
```