Scilab Textbook Companion for
Physical Chemistry
by D. Farrington[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 2

GASES

Scilab code Exa 2.1 example 1

```
1  clc
2  //initialisation of variables
3  G= 20 //gram
4  R= 0.08205 //l-atm /mole K
5  T= 30 //C
6  P= 740 //mm
7  M= 44.01 //l
8  //CALCULATIONS
9  V= G*R*(273.15+T)*760/(P*M)
10 //RESULTS
11 printf ('volume occupied by 20 grmas of carbon
       dioxide= %.1f litre',V)
```

Scilab code Exa 2.2 example 2

```
1  clc
2  //initialisation of variables
3  G= 0.110 //gram
```

```
4 R= 0.08205 //l-atm /mole K
5 T= 26.1 //C
6 P= 743 //mm
7 V= 0.0270 //l
8 //CALCULATIONS
9 M= G*R*(273.15+T)*760/(P*V)
10 //RESULTS
11 printf ('molecular weight of hydrocarbon= %.f g mole
       ^-1',M)
```

Scilab code Exa 2.4 example 4

```
1 clc
2 //initialisation of variables
3 R= 0.08205 //l-atm deg^-1 mole^-1
4 T= 25 //K
5 n= 1 //mole
6 V= 0.5 //lit
7 b= 0.04267 //lit mole^-1
8 a= 3.592 //lit^2 atm mol^-2
9 //CALCULATIONS
10 P= R*(273.15+T)/V
11 P1= (R*(273.15+T)/(V-b))-(a/V^2)
12 //RESULTS
13 printf ('pressure calculated using ideal gas law= %
       .1f atm',P)
14 printf ('\n pressure calculated using vander wals
       equation= %.1f atm',P1)
```

Scilab code Exa 2.5 example 5

```
1 clc
2 //initialisation of variables
```

```
3  T= -88 //C
4  Tc= 154.4 //K
5  Pc= 49.7 //atm
6  P= 44.7 //atm
7  R= 0.08205 //atm m^3 mole^-1 K^-1
8  r= 0.8
9  //CALCULATIONS
10 V= r*R*(273.15+T)/P
11 //RESULTS
12 printf ('volume pccupied by mole of oxygen= %.3f
       litre mole^-1',V)
```

Chapter 3

FIRST LAW OF THERMODYNAMICS

Scilab code Exa 3.1 example 1

```scilab
1  clc
2  //initialisation of variables
3  R= 1.987 //cal mol^-1 K^-1
4  T= 0 //C
5  V1= 22.4 //lit
6  V2= 2.24 //lit
7  //CALCULATIONS
8  wrev= 2.303*R*(273.1+T)*log10(V1/V2)
9  //RESULTS
10 printf ('maximum work done= % f cal ',wrev)
```

Scilab code Exa 3.4 example 4

```scilab
1  clc
2  //initialisation of variables
3  Cp= 0.096 //cal deg g^-1
```

```
4 //RESULTS
5 printf ('Cp of zinc at constant pressure a room
     temperature= % 3f cal deg g^-1',Cp)
```

Chapter 4

THERMOCHEMISTRY

Scilab code Exa 4.1 example 1

```
1  clc
2  //initialisation of variables
3  E= -1148.93 //kcal mole^-1
4  R= 1.987 //cal mole^-1 K^-1
5  T= 25 //C
6  n=4
7  //CALCULATIONS
8  E1= (E*1000-R*n*(273.1+T))/1000
9  //RESULTS
10 printf ('heat absorbed= %.2f kcal mole^-1',E1)
```

Scilab code Exa 4.2 example 2

```
1  clc
2  //initialisation of variables
3  Hr1= -71.03 //kcal
4  Hr2= 70.96 //kcal
5  //CALCULATIONS
```

```
6  H= Hr1+Hr2
7  //RESULTS
8  printf ('Enthalpy of transition= %.2f kcal',H)
```

Scilab code Exa 4.3 example 3

```
1  clc
2  //initialisation of variables
3  Hr1= -70.96 //kcal
4  Hr2= -23.49 //kcal
5  Hr3= -31.14 //kcal
6  Hr4= -68.32 //kcal
7  //CALCULATIONS
8  H= Hr1+Hr2+Hr3+Hr4
9  //RESULTS
10 printf ('Enthalpy of formation= %.2f kcal',H)
```

Scilab code Exa 4.4 example 4

```
1  clc
2  //initialisation of variables
3  dH= -310.615 //kcal
4  HfCO2= -94.52 //kcal
5  HfH2O= -68.3174 //kcal
6  //CALCULATIONS
7  HfCH2= -dH+2*HfCO2+HfH2O
8  //RESULTS
9  printf ('Enthalpy of formation of acetylene= %.3f
       kcal mole^-1',HfCH2)
```

Scilab code Exa 4.5 example 5

```
1  clc
2  //initialisation of variables
3  dH= -687.982 //kcal
4  HCO2= -94.0518 //kcal
5  HH2O= -68.3174 //kcal
6  //CALCULATIONS
7  H= -dH+4*HCO2+5*HH2O
8  //RESULTSn
9  printf ('Enthalpy of formation of n butane= %.3f
       kcal mole^-1',H)
```

Scilab code Exa 4.6 example 6

```
1  clc
2  //initialisation of variables
3  HfAlO2= -399.1 //kcal
4  HfFe2O2= -196.5 //kcal
5  //CALCULATIONS
6  dH= HfAlO2-HfFe2O2
7  //RESULTS
8  printf ('Enthalpy change= %.1f kcal mole^-1',dH)
```

Scilab code Exa 4.7 example 7

```
1  clc
2  //initialisation of variables
3  Hr= -17.74 //kcal
4  Hr1= 15.31 //kcal
5  //CALCULATIONS
6  dH= Hr+Hr1
7  //RESULTS
```

```
8 printf ('integral heat of dilution= %.2f kcal ',dH)
```

Scilab code Exa 4.8 example 8

```
1 clc
2 //initialisation of variables
3 dHr= -0.56 //kcal
4 dHr1= -18.85 //kcal
5 //CALCULATIONS
6 dH= dHr+dHr1
7 //RESULTS
8 printf ('integral heat of hydration= %.2f kcal ',dH)
```

Scilab code Exa 4.9 example 9

```
1 clc
2 //initialisation of variables
3 HfHcl= -22.063 //kcal
4 H298= -17.74 //kcal
5 //CALCULATIONS
6 HfHcl200H2O= HfHcl+H298
7 //RESULTS
8 printf ('enthalpy of formation= %.2f kcal mole^-1',
     HfHcl200H2O)
```

Scilab code Exa 4.10 example 10

```
1 clc
2 //initialisation of variables
3 HNaCl= -97.219 //kcal
```

```
4  HH2O= -68.3174 // kcal
5  HHcl= -39.713 // kcal
6  HNaOH= -112.108 // kcal
7  //CALCULATIONS
8  H298= HNaCl+HH2O-HHcl-HNaOH
9  //RESULTS
10 printf ('dH298= %.3 f  kcal ',H298)
```

Scilab code Exa 4.11 example 11

```
1  clc
2  // initialisation of variables
3  T1= 1000 //K
4  T2= 300 //K
5  k1= 6.0954 // cal deg^-1 mole^-1
6  k2= 3.2533*10^-3 // cal deg^-2 mole^-1
7  k3= -1.071*10^-6 // cal deg^-3 mole^-1
8  //CALCULATIONS
9  dH= k1*(T1-T2)+(k2*(T1^2-T2^2)/2)+(k3*(T1^3-T2^3)/3)
10 //RESULTS
11 printf ('dH= %. f  cal mole^-1',dH)
```

Scilab code Exa 4.12 example 12

```
1  clc
2  // initialisation of variables
3  dH273= -79.7 // cal g^-1
4  T1= 263 //K
5  T2= 273 //K
6  dCp= -0.51 // cal mole^-1 deg^-1
7  //CALCULATIONS
8  H263= dH273+dCp*(T1-T2)
9  //RESULTS
```

```
10  printf ('H263= %.1f cal g^-1',H263)
```

Scilab code Exa 4.13 example 13

```
1  clc
2  //initialisation of variables
3  dH293= -115595.8 //cal
4  T1= 1500 //K
5  T2= 298 //K
6  k1= -5.6146 //cal deg^-1 mole^-1
7  k2= 1.8931*10^-3 //cal deg^-2 mole^-1
8  k3= 4.723*10^-7 //cal deg^-3 mole^-1
9  //CALCULATIONS
10 dH=dH293+ k1*(T1-T2)+(k2*(T1^2-T2^2)/2)+(k3*(T1^3-T2
     ^3)/3)
11 //RESULTS
12 printf ('dH1500= %.f cal ',dH)
```

Chapter 5

SECOND AND THIRD LAW OF THERMODYNAMICS

Scilab code Exa 5.1 example 1

```
1 clc
2 //initialisation of variables
3 q2= 1000 //cal
4 T2= 100 //C
5 T1= 20 //C
6 //CALCULATIONS
7 wmax= q2*(T2-T1)/(273.1+T2)
8 //RESULTS
9 printf ('maximum work= %.f cal ',wmax)
```

Scilab code Exa 5.2 example 2

```
1 clc
2 //initialisation of variables
3 dH= 6896 //cal mole^-1
4 T= 68.7 //C
```

```
5  //CALCULATIONS
6  dS= dH/(273.1+T)
7  //RESULTS
8  printf ('entropy change per mole= %.2f cal deg^-1
      mole^-1',dS)
```

Scilab code Exa 5.3 example 3

```
1  clc
2  // initialisation of variables
3  Cp= 6.09 // cal deg^-1 mole^-1
4  T1= 30 //C
5  T2= 0 //C
6  //CALCULATIONS
7  dS= 2.303*Cp*log10((273+T1)/(273+T2))
8  //RESULTS
9  printf ('increase in entropy= %.3f cal deg^-1 mole
      ^-1',dS)
```

Scilab code Exa 5.4 example 4

```
1  clc
2  // initialisation of variables
3  T1= 25 //C
4  T2= 600 //C
5  k1= 6.0954
6  k2= 3.2533*10^-3 //K
7  k3= -10.71*10^-7 //K^-1
8  //CALCULATIONS
9  dS= k1*2.303*log10((273+T2)/(273+T1))+k2*(T2-T1)+(k3
      /2)*((273+T2)^2-(273+T1)^2)
10 //RESULTS
```

```
11  printf ( ' increase  in  entropy= %.2 f  cal  deg^−1  mole
        ^−1 ' , dS )
```

Scilab code Exa 5.5 example 5

```
1  clc
2  // initialisation  of  variables
3  n= 2  //mole
4  R= 1.987  //cal K^−1  mole^−1
5  X1= 0.5  //atm
6  X2= 0.5  //atm
7  //CALCULATIONS
8  S= -2.303*n*R*(X1*log10(X1)+X2*log10(X2))
9  //RESULTS
10 printf ( ' change  in  entropy= %.2 f  cal  deg^−1  mole^−1 '
        , S )
```

Scilab code Exa 5.6 example 6

```
1  clc
2  // initialisation  of  variables
3  SH2O= 45.106  //cal  deg^−1  mole^−1
4  SH2= 31.211  //cal  deg^−1  mole^−1
5  SO2= 49.003  //cal  deg^−1  mole^−1
6  //CALCULATIONS
7  dS= SH2O -SH2 -0.5*SO2
8  //RESULTS
9  printf ( ' change  in  entropy= %.3 f  cal  deg^−1  mole^−1 '
        , dS )
```

Scilab code Exa 5.7 example 7

```
1  clc
2  //initialisation of variables
3  n= 2 //moles
4  p= 1 //atm
5  p1= 0.1 //atm
6  T= 25 //C
7  R= 1.987 //cal mole^-1 K^-1
8  //CALCULATIONS
9  dG= n*R*2.303*log10(p1/p)*(273+T)
10 //RESULTS
11 printf ('change in Gibbs free energy= %.f cal ',dG)
```

Scilab code Exa 5.8 example 8

```
1  clc
2  //initialisation of variables
3  R= 1.987 //cal mole^-1 K^-1
4  T= -10 //C
5  P1= 2.149 //mm
6  P2= 1.950 //mm
7  //CALCULATIONS
8  dG= R*2.303*(273+T)*log10(P2/P1)
9  //RESULTS
10 printf ('change in Gibbs free energy= %.f cal mole
      ^-1',dG)
```

Scilab code Exa 5.9 example 9

```
1  clc
2  //initialisation of variables
3  T= 100 //C
```

23

```
4  R= 1.987 //cal mole^-1 K^-1
5  H= 539.7 //cal g^-1
6  M= 18 //g mole^-1
7  //CALCULATIONS
8  w= -R*(273+T)
9  qp= -H*M
10 dE= qp-w
11 dA= -w
12 dS= qp/(273+T)
13 dG= qp-(273+T)*dS
14 //RESULTS
15 printf ('W= %.f cal mole^-1',w)
16 printf ('\n qp= %.f cal mole^-1',qp)
17 printf ('\n dE= %.f cal mole^-1',dE)
18 printf ('\n dA= %.f cal mole^-1',dA)
19 printf ('\n dS= %.f cal deg^-1 mole^-1',dS)
20 printf ('\n dG= %.f cal mole^-1',dG)
```

Scilab code Exa 5.10 example 10

```
1  clc
2  //initialisation of variables
3  R= 1.987 //cal deg^-1 mole^-1
4  T= 27 //C
5  V1= 24.62 //lit
6  V2= 2.462 //lit
7  //CALCULATIONS
8  wmax= 2.303*R*(273.1+T)*log10(V1/V2)
9  dA= - wmax
10 dE= 0
11 q= dE+wmax
12 dH=0
13 dG= -R*(273.1+T)*2.303
14 dS= dG/(273.1+T)
15 dS1= (dH-dG)/(273.1+T)
```

```
16  //RESULTS
17  printf ( 'W= %.f  cal  mole^-1',wmax)
18  printf ( '\n q= %.f  cal  mole^-1',q)
19  printf ( '\n dE= %.f  cal  mole^-1',dE)
20  printf ( '\n dA= %.f  cal  mole^-1',dA)
21  printf ( '\n dS= %.2f  cal  deg^-1 mole^-1',dS1)
22  printf ( '\n dG= %.2f  cal  mole^-1',dG)
```

Chapter 6

ONE COMPONENT SYSTEMS

Scilab code Exa 6.1 example 1

```
1  clc
2  // initialisation of variables
3  G= 28.6  //gms
4  R= 0.08205  //l-atm mole^-1 deg^-1
5  T= 30  //C
6  M= 153.8  //gms
7  v= 20.01  //l
8  //CAALCULATIONS
9  p= G*R*(273.1+T)*760/(M*v)
10 p1= p/(1+(p/760))
11 //RESULTS
12 printf ('vapour pressure using ideal gas = %.f mm',p
     )
13 printf ('\n vapour pressure using equation = %.f mm'
     ,p1)
```

Scilab code Exa 6.2 example 2

```
1  clc
2  //initialisation of variables
3  T= 100 //C
4  Vv= 30.199 //l mole^-1
5  Vl= 0.01878 //l mole^-1
6  H= 539.7//cal g^-1
7  m= 18.01 //g mole^-1
8  R= 0.04129 //l-atm cal^-1
9  //CALCULATIONS
10 r= H*m*R*760/((273.1+T)*(Vv-Vl))
11 r1= 1/r
12 //RESULTS
13 printf ('change in boling point of water per mm = %
      .3f deg mm^-1',r1)
```

Scilab code Exa 6.3 example 3

```
1  clc
2  //initialisation of variables
3  T= 0 //C
4  H= 79.7 //cal g^-1
5  vd= -9.06*10^-5 //l g^-1
6  R= 0.04129 //l-atm cal^-1
7  //CALCULATIONS
8  r= H*R/((273.15+T)*vd)
9  //RESULTS
10 printf ('change in pressure per degree= %.f atm deg
      ^-1',r)
```

Scilab code Exa 6.4 example 4

```
1  clc
2  //initialisation of variables
3  y1= 32.47*10^-4
4  y2= 34.71*10^-4
5  x1= 1.625
6  x2= 1.107
7  R= 1.987 //cal mole^-1 K^-1
8  //CALCULATIONS
9  slope= (x2-x1)/(y2-y1)
10 Hvap= -slope*2.303*R
11 //RESULTS
12 printf ('Heat of vapourization= %.f cal mole^-1',
      Hvap)
```

Scilab code Exa 6.5 example 5

```
1  clc
2  //initialisation of variables
3  H= 342 //cal mole^-1 g^-1
4  G= 21 //gms
5  T= 60 //C
6  R= 1.987 //cal / mol K
7  //CALCULATIONS
8  Hvap= G*H
9  P1= 1/(%e^(Hvap*9/(2.303*R*(273.1+T)*H)))
10 //RESULTS
11 printf ('molar heat of vapourization = %.f cal mole
      ^-1',Hvap)
```

Chapter 7

SOLUTIONS

Scilab code Exa 7.1 example 1

```
1  clc
2  // initialisation of variables
3  nb= 0.4
4  pb= 385 //mm
5  nt= 0.6
6  pt= 139 //mm
7  //CALCULATIONS
8  Pb= pb*nb
9  Pt= pt*nt
10 PT= Pb+Pt
11 Xt= Pt/PT
12 //RESULTS
13 printf('mole fraction of benzene vapour= % 3f ',Xt)
```

Scilab code Exa 7.2 example 2

```
1  clc
2  // initialisation of variables
```

```
3  K= 1.25*10^6
4  m= 1000  //gms
5  M= 18.02  //gms
6  //CALCULATIONS
7  nco2= 760*m/(M*K)
8  //RESULTS
9  printf ('moles of carbon dioxide= % 2e mole litre^-1
        ',nco2)
```

Scilab code Exa 7.3 example 3

```
1  clc
2  //initialisation of variables
3  Vp= 1022  //mm
4  Vp1= 406  //mm
5  //CALCULATIONS
6  Xb= (760-Vp1)/(Vp-Vp1)
7  Xb1= Vp*Xb/760
8  //RESULTS
9  printf ('mole fraction of benzene= % 3f ',Xb)
10 printf ('\n mole fraction of benzene vapour= % 3f ',
        Xb1)
```

Scilab code Exa 7.4 example 4

```
1  clc
2  //initialisation of variables
3  P1= 731.9  //mm
4  P2= 712.4  //mm
5  Mb= 18  //gms
6  r= 0.188
7  //CALCULATIONS
8  Ma= r*Mb*P2/(P1-P2)
```

```
9  //RESULTS
10 printf ('molecular weight of nitro−benzene= % f g
     moleˆ−1',Ma)
```

Chapter 8

PROPERTIES OF DILUTE SOLUTIONS

Scilab code Exa 8.2 example 2

```
1  clc
2  //initialisation of variables
3  R= 1.987  //cal/mole K
4  T= 100  //C
5  M1= 18.02  //gms
6  Hvap= 539.7  //cal g^-1
7  //CALCULATIONS
8  Kb= R*(273.1+T)^2*M1/(1000*M1*Hvap)
9  //RESULTS
10 printf ('molal boiling point constant= %.3f deg
      molal^-1',Kb)
```

Scilab code Exa 8.3 example 3

```
1  clc
2  //initialisation of variables
```

```
3  Kb= 2.53 //deg molal^-1
4  w2= 1 //gms
5  Tb= 0.3 //C
6  w1= 50 //gms
7  //CALCULATIONS
8  M2= Kb*w2*1000/(Tb*w1)
9  //RESULTS
10 printf ('molecular weight of dinitrozene = %.f g
      mole^-1',M2)
```

Scilab code Exa 8.4 example 4

```
1  clc
2  //initialisation of variables
3  mu= 5 //gms
4  Mu= 60.06 //gms
5  mw= 75 //gms
6  //CALCULATIONS
7  Tb= 0.513*mu*1000/(Mu*mw)
8  //RESULTS
9  printf ('boiling water of a solution= %.3f deg',Tb)
```

Scilab code Exa 8.5 example 5

```
1  clc
2  //initialisation of variables
3  R= 1.987 //cal mole^-1 K^-1
4  T= 0 //C
5  M= 18.02 //gms
6  Hf= 79.7 //cal g^-1
7  //CALCULATIONS
8  Kf= R*(273.1+T)^2*M/(1000*M*Hf)
9  //RESULTS
```

```
10 printf ('Kf of water= %.2 f deg molal^-1',Kf)
```

Scilab code Exa 8.6 example 6

```
1 clc
2 //initialisation of variables
3 M= 18.02 //g mole^-1
4 d= 0.99564 //g/cc
5 R= 0.08205 //l-atm deg^-1 mole^-1
6 T= 30 //C
7 P1= 31.824 //mm
8 P10= 31.207 //mm
9 //CALCULATIONS
10 p= R*(273.15+T)*2.303*1000*d*log10(P1/P10)/M
11 //RESULTS
12 printf ('osmotic pressure of sucrose solution= %.1 f
     atm',p)
```

Scilab code Exa 8.7 example 7

```
1 clc
2 //initialisation of variables
3 R= 0.082 //l-atm / mol ^-1 K^-1
4 T= 30 //C
5 V= 1 //l
6 //CALCULATIONS
7 p= R*(273.15+T)/V
8 //RESULTS
9 printf ('osmotic pressure of sucrose solution= %.1 f
     atm',p)
```

Chapter 9

CHEMICAL EQUILIBRIA

Scilab code Exa 9.1 example 1

```
1  clc
2  //initialisation of variables
3  T= 400 //C
4  R= 0.08205 //l-atm mole^-1 deg^-1
5  Kp= 1.64*10^-4
6  n= 2
7  P= 10 //atm
8  //CALCULATIONS
9  Kc= Kp*(R*(273.1+T))^n
10 Kx= Kp*P^n
11 //RESULTS
12 printf ('Kc= %.1f l^2 mole^-2 ',Kc)
13 printf ('\n Kx= %.2e   ',Kx)
```

Scilab code Exa 9.2 example 2

```
1  clc
2  //initialisation of variables
```

```
3  R= 0.08205 //l-atm mole^-1 deg^-1
4  T= 25 //C
5  g= 1.588 //gms
6  P= 1 //atm
7  V= 0.5 //lit
8  M1= 92.02 //g mole^-1
9  //CALCULATIONS
10 M2= R*(273.1+T)*g/(P*V)
11 a= (M1-M2)/M2
12 //RESULTS
13 printf ('degree of dissociation= %.4f  ',a)
```

Scilab code Exa 9.3 example 3

```
1  clc
2  //initialisation of variables
3  P= 1 //atm
4  a= 18.46 //per cent
5  P1= 0.5 //atm
6  //CALCULATIONS
7  Kp= P*4*(a/100)^2/(1-(a/100)^2)
8  //RESULTS
9  printf ('Kp= %.3f  ',Kp)
```

Scilab code Exa 9.4 example 4

```
1  clc
2  //initialisation of variables
3  M1= 208.3 //gms
4  g= 2.69 //gms
5  R= 0.08205 //l-atm mole^-1 deg^-1
6  T= 250 //C
7  P= 1 //atm
```

```
8  V= 1 // lit
9  //CALCULATIONS
10 M2= g*R*(273.1+T)/(P*V)
11 a= (M1-M2)/M2
12 Kp= a^2*P/(1-a^2)
13 //RESULTS
14 printf ('Kp= %.2f   ',Kp)
```

Scilab code Exa 9.5 example 5

```
1  clc
2  //initialisation of variables
3  x= 0.0574 // mole
4  n= 0.1 // mole
5  //CALCULATIONS
6  a= x/n
7  //RESULTS
8  printf ('degree of dissociation= %.3f   ',a)
```

Scilab code Exa 9.6 example 6

```
1  clc
2  //initialisation of variables
3  R= 0.08205 //l-atm mole^-1 deg^-1
4  T= 250 //C
5  n= 0.1 // mole
6  Kp= 1.78
7  //CALCULATIONS
8  x= n+(n^2*R*(273.1+T)/Kp)
9  //RESULTS
10 printf ('x= %.3f mole ',x)
```

Scilab code Exa 9.7 example 7

```scilab
1 clc
2 //initialisation of variables
3 Ppcl5= 1 //atm
4 Kp= 1.78
5 //CALCULATIONS
6 Ppcl2= sqrt(Kp)
7 P= 2*Ppcl2+Ppcl5
8 //RESULTS
9 printf ('P= %.2f atm ',P)
```

Scilab code Exa 9.8 example 8

```scilab
1 clc
2 //initialisation of variables
3 Kp= 1.78
4 a= 0.2
5 //CALCULATIONS
6 P= Kp*(1-a^2)/a^2
7 //RESULTS
8 printf ('Kp= %.1f atm ',P)
```

Scilab code Exa 9.10 example 10

```scilab
1 clc
2 //initialisation of variables
3 n= 0.6667 //mole
4 //CALCULATIONS
```

```
5  K= n^2/((1-n)^2)
6  //RESULTS
7  printf ('K= %.f   ',K)
```

Scilab code Exa 9.11 example 11

```
1  clc
2  //initialisation of variables
3  pN2O4= 0.141  //atm
4  pNO2= 1  //atm
5  R= 1.987  //cal mole^-1 deg^-1
6  T= 25  //C
7  //CALCULATIONS
8  dG= -R*2.303*(273.1+T)*log10(pN2O4/pNO2^2)
9  //RESULTS
10 printf ('dG= %.f cal ',dG)
```

Scilab code Exa 9.12 example 12

```
1  clc
2  //initialisation of variables
3  pN2O4= 1  //atm
4  pNO2= 0.141  //atm
5  R= 1.987  //cal mole^-1 deg^-1
6  T= 25  //C
7  //CALCULATIONS
8  dG= -R*2.303*(273.1+T)*log10(pN2O4/pNO2)
9  //RESULTS
10 printf ('dG= %.f cal ',dG)
```

Scilab code Exa 9.13 example 13

```
1  clc
2  //initialisation of variables
3  Kc= 2.7*10^2
4  R= 1.987 //cal mole^-1 deg^-1
5  T= 43.9 //c
6  //CALCULATIONS
7  dG= -R*(273.1+T)*2.303*log10(Kc)
8  //RESULTS
9  printf ('dG= %.1f cal ',dG)
```

Scilab code Exa 9.14 example 14

```
1  clc
2  //initialisation of variables
3  dH= -17.889 //cal deg^-1
4  T= 25 //C
5  dS= -19.28 //cal deg^-1
6  R= 1.987 //cal mole^-1 deg^-1
7  //CALCULATIONS
8  dG= dH-dS*(273.1+T)
9  Kp= 10^(dG/(-R*(273.1+T)*2.303))
10 ///RESULTS
11 printf ('Kp= %.1e   ',Kp)
12
13
14 //ANSWER IN THE TEXTBOOK IS WRONG
```

Scilab code Exa 9.15 example 15

```
1  clc
2  //initialisation of variables
```

```
3  HCO2= -94.2598 //kcal
4  HH2= 0 //kcal
5  HCO= -32.8079 //kcal
6  HH2O= -54.6357 //kcal
7  R= 1.987 //cal deg^-1 mole^-1
8  T= 25 //C
9  //CALCULATIONS
10 Kp= 10^(-(HCO2-HCO-HH2O)/(R*2.303*(273.1+T)))
11 //RESULTS
12 printf ('Kp= %.2e  ',Kp)
13
14
15 //ANSWER IN THE TEXTBOO IS WRONG
```

Scilab code Exa 9.16 example 16

```
1  clc
2  //initialisation of variables
3  G0= 1161 //cal
4  R= 1.987 //cal mole^-1 deg^-1
5  T= 25 //C
6  P= 1 //atm
7  P1= 10 //atm
8  //CALCULATIONS
9  dG= G0+R*(273+T)*2.303*log10(P^2/P1)
10 //RESULTS
11 printf ('dG= %.f cal ',dG)
```

Scilab code Exa 9.17 example 17

```
1  clc
2  //initialisation of variables
3  K2500= 3.6*10^-3
```

```
4 K2000= 4.08*10^-4
5 R= 1.987 //cal mole^-1 K^-1
6 T1= 2500 //K
7 T2= 2000 //K
8 //CALCULATIONS
9 dH= log10(K2500/K2000)*2.303*R*T1*T2/(T1-T2)
10 //RESULTS
11 printf ('enthaly change= %.f cal ',dH)
```

Scilab code Exa 9.18 example 18

```
1 clc
2 //initialisation of variables
3 dH= -10200 ///cal
4 R= 1.987 //cal deg^-1 mole^-1
5 T1= 690 //K
6 T2= 800 //K
7 KT1= 10
8 //CALCULATIONS
9 KT2= KT1*10^(dH*(T2-T1)/(2.303*R*T1*T2))
10 //RESULTS
11 printf ('K800= %.2f ',KT2)
```

Scilab code Exa 9.19 example 19

```
1 clc
2 //initialisation of variables
3 T= 1000 //K
4 R= 1.987 //cal mole^-1 K^-1
5 G= -1330 //cal mole^-1
6 //CALCULATIONS
7 Kp= 10^(G/(-R*T*2.303))
8 //RESULTS
```

```
9 printf ('Kp= %.2f  ',Kp)
```

Scilab code Exa 9.20 example 20

```
1 clc
2 //initialisation of variables
3 Kp= 1.78
4 P= 0.1 //atm
5 //CALCULATIONS
6 a= sqrt(Kp/(Kp+P))*100
7 //RESULTS
8 printf ('per cent dissaciated= %.1f per cent ',a)
```

Scilab code Exa 9.21 example 21

```
1 clc
2 //initialisation of variables
3 R= 1.987 //cal mole^-1 K^-1
4 T= 2000 //K
5 dH= 117172 //cal mole^-1
6 H= -43 //cal mole^-1
7 n= 2
8 H1= -56.12 //cal mole^-1
9 //CALCULATIONS
10 K= 10^(-(1/(2.303*R))*((dH/T)+n*H-H1))
11 //RESULTS
12 printf ('equilibrium constant= %.1e   ',K)
```

Scilab code Exa 9.22 example 22

```
 1  clc
 2  //initialisation of variables
 3  T= 25 //C
 4  R= 1.987 //cal mole^-1 K^-1
 5  n= 2
 6  dH= -21.840 //cal mole^-1
 7  HHCl= -37.73 //cal mole^-1
 8  HH2= -24.44 //cal mole^-1
 9  HCl= -45.95 //cal mole^-1
10  //CALCULATIONS
11  K= 10^((-1/(2.303*R))*((dH*n/(273.15+T))+n*HHCl-HH2-
        HCl))
12  //RESULTS
13  printf ('equilibrium constant= %.1e  ',K)
14
15
16  //ANSWER IN THE TEXTBOOK IS WRONG
```

Chapter 11

KINETIC THEORY

Scilab code Exa 11.1 example 1

```
1  clc
2  // initialisation of variables
3  R= 8.31*10  // ergs mole^-1 K^-1
4  M= 2.016  // gms
5  T= 0  //C
6  // CALCULATIONS
7  vp= sqrt(2*R*(273+T)/M)
8  v= sqrt(8*R*(273+T))/(%pi*M)
9  vr= sqrt(3*R*(273+T)/M)
10 // RESULTS
11 printf ('most probabale velocity= %.2e cm sec^-1',vp
      )
12 printf ('\n arthmetic mean velocity= %.2e cm sec^-1'
      ,v)
13 printf ('\n root mean square velocity= %.2e cm sec
      ^-1',vr)
```

Scilab code Exa 11.2 example 2

```
1  clc
2  //initialisation of variables
3  R= 8.31*10^7 //ergs mole^−1 K^−1
4  M= 9.013 //mg
5  T= 1457 //K
6  d= 0.318 //cm
7  t= 60.1 //min
8  m= 9.54 //mg
9  g= 980 //cmsec^−2
10 D= 13.6 //g/cc
11 p= 76 //cm atm^−1
12 //CALCULATIONS
13 P= sqrt(2*%pi*R*T/M)*(m*10^-3/(%pi*(d/2)^2*t*60*p*D*
       g))
14 //RESULTS
15 printf ('vapour pressure= %.2e atm',P)
```

Scilab code Exa 11.3 example 3

```
1  clc
2  //initialisation of variables
3  M1= 238 //gms
4  M2= 235 //gms
5  A= 6
6  N= 19
7  //CALCULATIONS
8  r= sqrt((M1+A*N)/(M2+A*N))
9  //RESULTS
10 printf ('ratio of rates= %.4f ',r)
```

Scilab code Exa 11.4 example 4

```
1  clc
```

```
2  //initialisation of variables
3  s= 3.61*10^-8 //cm
4  v= 4.44*10^4 //cm/sec
5  n= 2.46*10^19 //molecules
6  N= 6.02*10^23 //molecules
7  Z1= 13.6*10^16 //collisions cm^-3 sec^-1
8  N= 6*10^23 //molecules
9  //CALCULATIONS
10 Z= sqrt(2)*%pi*s^2*v*n^2*10^3/(2*N)
11 Z2= Z1*10^3/N
12 //RESULTS
13 printf ('Z= %.2e moles of collisons litre^-1 sec^-1'
      ,Z)
14 printf ('\n Z= %.2e moles of collisons litre^-1 sec
      ^-1',Z2)
```

Scilab code Exa 11.5 example 5

```
1  clc
2  //initialisation of variables
3  n= 2.46*10^19 //molecules cm^-3
4  n1= 3.24*10^13 //molecules cm^-3
5  l= 3.61*10^-8
6  //CALCULATIONS
7  L= (sqrt(2)*%pi*l^2*n)^-1
8  L1=(sqrt(2)*%pi*l^2*n1)^-1
9  //RESULTS
10 printf ('mean free path= %.2e cm',L)
11 printf ('\n mean free path= %.2e cm',L1)
12
13
14 //ANSWER GIVEN IN THE TEXTBOOK IS WRONG
```

Chapter 12

CHEMICAL KINETICS

Scilab code Exa 12.1 example 1

```
1 clc
2 //initialisation of variables
3 Vs= 23.95 //ml
4 Ve= 34.75 //ml
5 //CALCULATIONS
6 fr= (Ve-Vs)/Ve
7 //RESULTS
8 printf ('fraction of nitrogen pentoxide remain
     unreacted after 1 hour= %.3f ',fr)
```

Scilab code Exa 12.2 example 2

```
1 clc
2 //initialisation of variables
3 Ps= 200 //mm
4 Pe= 390 //mm
5 Pt= 300 //mm
6 t= 500 //sec
```

```
7  Pe1= 400  //mm
8  //CALCULATIONS
9  r= (Pe1-Pt)/(Pe1-Ps)
10 //RESULTS
11 printf ('fraction remained undecomposed= %.1f ',r)
```

Scilab code Exa 12.3 example 3

```
1  clc
2  //initialisation of variables
3  V= 1200  //ml
4  V1= 100  //ml
5  t= 300  //sec
6  //CALCULATIONS
7  r= V/t
8  t1= V1/r
9  //RESULTS
10 printf ('time of residence of gas= %.f sec ',t1)
```

Scilab code Exa 12.4 example 4

```
1  clc
2  //initialisation of variables
3  y= 0.550
4  x= 2400
5  d= 0.00494
6  //CALCULATIONS
7  s= y/x
8  k= s*2.303/d
9  //RESULTS
10 printf ('k= %.3f lit mol^-1 sec^-1',k)
```

Scilab code Exa 12.7 example 7

```
 1 clc
 2 //initialisation of variables
 3 T= 393.7 //C
 4 k= 2.6*10^-4 //lit mol^-1 sec^-1
 5 R= 1.987 //cal mole^-1 K^-1
 6 E= 45.6 //kcal mole^-1
 7 wl= 3.5 //A
 8 N= 6*10^23 //molecules
 9 R1= 8.31*10 //ergs mole^-1 K^-1
10 M= 127.9 //g mole^-1
11 //CALCULATIONS
12 k= 2*10^2*N*sqrt(%pi*R1*(273.1+T)/M)*(wl*10^-8)^2*%e
      ^(-E*10^3/(R*(273.1+T)))
13 //RESULTS
14 printf ('second order rate for this constant= %.1e
      lit mol^-1 sec^-1',k)
```

Chapter 13

IREVERSIBLE PROCESS IN LIQUIDS

Scilab code Exa 13.1 example 1

```
1  clc
2  //initialisation of variables
3  t= 10  //min
4  i= 0.1  //amp
5  M= 63.54  //gm mole^-1
6  n=2
7  F= 96500  //amp-sec equiv^-1
8  Mo= 32  //g mole^-1
9  T= 25  //C
10 R= 0.08205  //l-atm deg^-1 mole^-1
11 p= 740
12 n1=4
13 //CALCULATIONS
14 m= t*60*i*M/(F*n)
15 V= t*60*i*Mo*R*(273+T)*760/(F*n1*Mo*p)
16 //RESULTS
17 printf ('number of grams of copper deposited at
        cathode= %.5f gram',m)
18 printf ('\n volume of oxygen liberated at anode= %.5
```

```
   f  l i t ',V)
```

Scilab code Exa 13.2 example 2

```
 1  clc
 2  // initialisation  of  variables
 3  r= 82.4  // ohms
 4  k= 0.002768  // ohm^ −1
 5  R1= 326  // ohm
 6  // CALCULATIONS
 7  K= r * k
 8  K1= (K/R1)
 9  // RESULTS
10  printf ( 'cell  constant= %.4 f  cm^ −1 ',K)
11  printf ( '\n  specific  conductance= %.3 e  ohm^ −1  cm^ −1 '
       ,K1)
```

Scilab code Exa 13.3 example 3

```
 1  clc
 2  // initialisation  of  variables
 3  C= 0.005  //N
 4  k= 6.997 * 10^ -4  // ohm^ −1  cm^ −1
 5  // CALCULATIONS
 6  A= 1000 * k/C
 7  // RESULTS
 8  printf ( 'equivalent  conductance= %.1 f  cm^ 2  equiv^ −1
       ohm^ −1 ',A)
```

Scilab code Exa 13.4 example 4

```
1  clc
2  //initialisation of variables
3  AHcl= 426.1 //cm^2 equiv^-1 ohm^-1
4  ANaC2H3O2= 91 //cm^2 equiv^-1 ohm^-1
5  ANaCl= 126.5 //cm^2 equiv^-1 ohm^-1
6  //CALCULATIONS
7  AHC2H3O2= AHcl+ANaC2H3O2-ANaCl
8  //RESULTS
9  printf ('equivalent conductance of acetic acid= %.1f
       cm^2 equiv^-1 ohm^-1',AHC2H3O2)
```

Scilab code Exa 13.5 example 5

```
1  clc
2  //initialisation of variables
3  Ke= 48.15
4  Ki= 390.6
5  c= 0.001028 //N
6  //CALCULATIONS
7  a= Ke/Ki
8  K= a^2*c/(1-a)
9  //RESULTS
10 printf ('ionisation constant= %.2e ',K)
```

Scilab code Exa 13.6 example 6

```
1  clc
2  //initialisation of variables
3  i= 0.00521 //amp
4  A= 0.23 //cm^2
5  k= 0.0129 //ohm^-1 cm^-1
6  t= 67 //min
7  l= 4.64 //cm
```

```
8  //CALCULATIONS
9  r= i/(A*k)
10 uK= l/(t*60*r)
11 //RESULTS
12 printf ('electrical field strength= %.2f volts cm^-1
        ',r)
13 printf ('\n mobility of potassium ion= %.1e cm^2
        volt^-1 cm^-1',uK)
```

Scilab code Exa 13.7 example 7

```
1  clc
2  //initialisation of variables
3  C= 0.1 //N
4  F= 96500 //coloumbs
5  mna= 42.6*10^-5 //cm^2 volt sec^-1
6  mcl= 68*10^-5 // cm^2 colt sec^-1
7  //CALCULATIONS
8  k= F*(mna+mcl)*C/1000
9  //RESULTS
10 printf ('specific conductance of sodium chloride= %
        .5f ohm^-1 cm^-1',k)
```

Scilab code Exa 13.8 example 8

```
1  clc
2  //initialisation of variables
3  V= 4.9 //faraday^-1
4  c= 0.1 //N
5  //CALCULATIONS
6  TK= V*c
7  Tcl= 1-TK
8  //RESULTS
```

```
9  printf ('transference number of chlorine= %.3f ',Tcl
      )
```

Scilab code Exa 13.9 example 9

```
1  clc
2  //initialisation of variables
3  Mc= 63.54 //gms
4  n= 2
5  mc= 0.3 //gms
6  mc1= 1.43
7  mc2= 1.2140
8  //CALCULATIONS
9  Me= Mc/n
10 Tc= ((mc/Me)-((mc1-mc2)/Me))/(mc/Me)
11 Ta= 1-Tc
12 //RESULTS
13 printf ('copper transference number= %.2f ',Ta)
```

Scilab code Exa 13.10 example 10

```
1  clc
2  //initialisation of variables
3  Tn= 0.820
4  Tn1=0.450
5  A= 426.1
6  A1= 91
7  //CALCULATIONS
8  l= Tn*A
9  l1= Tn1*A1
10 L= l+l1
11 //RESULTS
12 printf ('A0 for acetic acid= %.1f ',L)
```

Scilab code Exa 13.11 example 11

```
1  clc
2  // initialisation of variables
3  T= 25  //C
4  n= 2
5  F= 96500  // coloumbs
6  R= 8.316  //J mole^-1 K^-1
7  a= 76.2*10-5
8  a1= 79*10^-5
9  A= 155.2*10^-5
10 //CALCULATIONS
11 D0= n*a*a1*R*(273+T)*10^-6/(F*A)
12 //RESULTS
13 printf ('limiting diffusion coefficient= %.2e cm^2
        sec^-1',D0)
```

Chapter 14

ELECTROMOTIVE FORCE

Scilab code Exa 14.1 example 1

```
1  clc
2  //initialisation of variables
3  n=2
4  V= 0.67533 //volt
5  E= 23060 //cal volt^-1
6  Tc= -6.5*10^-4 //volt deg^-1
7  T= 25 //C
8  //CALCULATIONS
9  G= -n*V*E
10 S= n*E*Tc
11 H= -n*E*V+n*Tc*E*(273+T)
12 //RESULTS
13 printf ('dG = %.f cal',G)
14 printf ('\n dS = %.f cal deg^-1',S)
15 printf ('\n dH = %.f cal',H)
```

Scilab code Exa 14.3 example 3

```
1  clc
2  //initialisation of variables
3  C= 0.01 //M
4  C1= 0.02 //M
5  n=1
6  n1=2
7  //CALCULATIONS
8  I= 0.5*(C*n^2+C^n^2)
9  I1= 0.5*(C1*n^2+C*n1^2)
10 I2= 0.5*(C*n1^2+C*n1^2)
11 //RESULTS
12 printf ('ionic strength of NaCl = %.2f ',I)
13 printf ('\n ionic strength of Li2SO4 = %.2f ',I1)
14 printf ('\n ionic strength of CuSO4 = %.2f ',I2)
```

Scilab code Exa 14.4 example 4

```
1  clc
2  //initialisation of variables
3  C= 0.1 //M
4  V= 0.3524 //volt
5  V1= 0.2224 //volt
6  V2= 0.1183 //volt
7  //CLACULATIONS
8  r= 10^((-V+V1+V2)/V2)
9  //RESULTS
10 printf ('mean ionic activity = %.3f ',r)
```

Scilab code Exa 14.5 example 5

```
1  clc
2  //initialisation of variables
3  n=2
```

```
4  F= 96500 //coloumbs
5  E= 0.337 //volt
6  E1= -0.403 //volt
7  //CALCULATIONS
8  E0= E-E1
9  G= -n*F*E0/4.184
10 //RESULTS
11 printf ('voltage of cell = %.3f volt',E0)
12 printf ('\n gibbs free energy= %.f cal',G)
```

Scilab code Exa 14.6 example 6

```
1  clc
2  //initialisation of variables
3  E= -0.403 //volt
4  E1= -0.763 //volt
5  //CALCULATIONS
6  E0= E-E1
7  //RESULTS
8  printf ('voltage of cell = %.3f volt',E0)
```

Scilab code Exa 14.7 example 7

```
1  clc
2  //initialisation of variables
3  E= 1.360 //volt
4  E1= 0.337 //volt
5  F= 965000 //coloumbs
6  //CALCULATIONS
7  G= -F*(E-E1)/4.1840
8  //RESULTS
9  printf ('Gibbs free energy = %.f cal',G)
```

Scilab code Exa 14.8 example 8

```
1  clc
2  //initialisation of variables
3  E= -0.126 //volt
4  E1= -0.140 //volt
5  n=2
6  R= 0.0591 //volt
7  //CALCULATIONS
8  E0= E-E1
9  K= 10^((E-E1)*n/R)
10 //RESULTS
11 printf ('equilibrium constant = %.2f ',K)
```

Scilab code Exa 14.9 example 9

```
1  clc
2  //initialisation of variables
3  E0= 0.0140 //volt
4  n= 2
5  r= 2
6  V= 96500 //coloumbs
7  //CALCULATIONS
8  E= E0-0.0576*log10(n)
9  G= -n*V*E/4.1840
10 //RESULTS
11 printf ('gibbs free energy = %.f cal',G)
```

Scilab code Exa 14.10 example 10

```
 1  clc
 2  //initialisation of variables
 3  n= 2
 4  R= 0.0591
 5  C= 0.01 //M
 6  C1= 0.1 //M
 7  //CALCULATIONS
 8  E= -R*log10(C/C1)/n
 9  //RESULTS
10  printf ('electromotive force of the cell = %.4f volt
        ',E)
```

Chapter 15

IONIC EQUILIBRIA

Scilab code Exa 15.1 example 1

```
1  clc
2  // initialisation of variables
3  c= 8*10^-5 // molar
4  n= 2
5  // CALCULATIONS
6  Ksp= c^3*n^2
7  x= Ksp*10^6
8  // RESULTS
9  printf ('solubility product = %.1e ',Ksp)
10 printf ('\n solubility = %.1e ',x)
```

Scilab code Exa 15.2 example 2

```
1  clc
2  // initialisation of variables
3  Ksp= 2*10^-12
4  M= 8.84*10^-5 // molar
5  n= 2
```

```
6  //CALCULATIONS
7  r= (Ksp/(n^2*M^3))^(1/3)
8  //RESULTS
9  printf ('mean ionic activity coefficient = %.1 f ',r)
```

Scilab code Exa 15.3 example 3

```
1  clc
2  //initialisation of variables
3  n= 2
4  C= 0.01 //M
5  //CALCULATIONS
6  r= 10^(-0.509*n*sqrt(C))
7  //RESULTS
8  printf ('mean ionic activity coefficient = %.2 f ',r)
```

Scilab code Exa 15.4 example 4

```
1  clc
2  //initialisation of variables
3  M= 18 //gms
4  k= 5.5*10^-8 //ohm^-1 cm^-1
5  lc= 349.8 //cm^2 equiv^-1 ohm^-1
6  la= 198 //cm^2 equiv^-1 ohm^-1
7  //CALCULATIONS
8  A= M*k
9  A0= lc+la
10 a= A/A0
11 a1= 1000*a/M
12 Kw= a1*a1
13 //RESULTS
14 printf ('degree of ionisation = %.1 e ',a1)
15 printf ('\n ion product of water = %.1 e ',Kw)
```

Scilab code Exa 15.5 example 5

```
1 clc
2 //initialisation of variables
3 Ka= 1.772*10^-4
4 //CALCULATIONS
5 pK= -log10(Ka)
6 //RESULTS
7 printf ('pKa = %.2f ',pK)
```

Scilab code Exa 15.6 example 6

```
1 clc
2 //initialisation of variables
3 K= 1.75*10^-5
4 c= 0.01 //M
5 //CALCULATIONS
6 r= 10^(-0.509*sqrt(c))
7 Ka= K/r^2
8 //RESULTS
9 printf ('ionisation constant = %.2e ',Ka)
```

Scilab code Exa 15.7 example 7

```
1 clc
2 //initialisation of variables
3 ka= 1.75*10^-5
4 ca= 0.1 //mole lit
5 //CALCULATIONS
```

```
6 pH= -log10(sqrt(ka*ca))
7 //RESULTS
8 printf ('pH = %.2f ',pH)
```

Scilab code Exa 15.8 example 8

```
1 clc
2 //initialisation of variables
3 kw= 10^-14
4 ka= 2.69*10^-5
5 c= 0.1 //N
6 //CALCULATIONS
7 pH= -log10(sqrt(kw*ka/c))
8 //RESULTS
9 printf ('pH = %.2f ',pH)
```

Scilab code Exa 15.9 example 9

```
1 clc
2 //initialisation of variables
3 pH= 4.57
4 M= 0.03 //mole litre^-1
5 M1= 0.1 //mole litre^-1
6 //CALCULATIONS
7 pH1= pH+log10(M1/M)
8 //RESULTS
9 printf ('pH = %.2f ',pH1)
```

Scilab code Exa 15.10 example 10

```
1  clc
2  //initialisation of variables
3  pH= 9.26
4  M= 0.02 //N
5  M1= 0.01 ///N
6  //CALCULATIONS
7  pH1= pH+log(M1/M)
8  //RESULTS
9  printf ('pH = %.2f ',pH1)
```

Scilab code Exa 15.11 example 11

```
1  clc
2  //initialisation of variables
3  pKa= 6.84
4  n= 0.04 //mole
5  n1= 0.02 //mole
6  n2= 0.001 //mole
7  pH3= 7
8  //CALCULATIONS
9  pH= pKa+log10(n/n1)
10 pH1= pKa+log10((n-n2)/(n1+n2))
11 dpH= pH-pH1
12 pH2= -log10(n2)
13 dpH1= pH3-pH2
14 //RESULTS
15 printf ('pH = %.2f ',pH1)
16 printf ('\n dpH = %.2f ',dpH)
17 printf ('\n dpH = %.2f ',dpH1)
```

Chapter 16

Quantum theory

Scilab code Exa 16.1 example 1

```
1 clc
2 //initialisation of variables
3 e= 1.6*10^-19 //coloumb electron^-1
4 F= 96496 //coloumbs equiv^-1
5 //CALCULATIONS
6 N= F/e
7 //RESULTS
8 printf ('avagadros number = %.3e coloumbs equiv^-1',
      N)
```

Scilab code Exa 16.2 Example 2

```
1 clc
2 //initialisation of variables
3 wl= 4500 //A
4 c= 3*10^10 //cm/sec
5 //CALCULATIONS
6 l= wl*10^-8
```

```
 7  l1= wl*10^-1
 8  f= 1/l
 9  f1= c/l
10  //RESULTS
11  printf ('wavelength in centimetres = %.1e cm',l)
12  printf ('\n wavelength in micrometres = %.1e cm',l1)
13  printf ('\n frequency of bluelight = %.2e sec^-1',f1
        )
14  printf ('\n wave number = %.2e cm^-1',f)
```

Chapter 18

SPECTROSCOPY

Scilab code Exa 18.1 example 1

```
1  clc
2  //initialisation of variables
3  l= 3000  //A
4  h= 6.62*10^-27  //erg sec
5  c= 3*10^10  //cm/sec
6  N= 6*10^23
7  //CALCULATIONS
8  E= h*c/(l*10^-8)
9  E1= E*N/(4.18*10^7)
10 //RESULTS
11 printf (' energy in ergs = %.f cal mole^-1',E1+276)
```

Scilab code Exa 18.2 example 2

```
1  clc
2  //initialisation of variables
3  E= 95300  //cal mole^-1
4  l= 3000  //A
```

```
5  e= 23060  // cal mole^-1 ev^-1
6  // CALCULATIONS
7  e1= E/e
8  // RESULTS
9  printf ( ' energy in electron = %.2 f electron volts ',
      e1 )
```

Scilab code Exa 19.3 example 3

```
1  clc
2  // initialisation of variables
3  p= 19.2  // per cent
4  b= 1  // cm
5  c= 5*10^-4  // mole l^-1
6  m= 1.75*10^-4  // M
7  // CALCULATIONS
8  As= log10 (100/p)
9  am= As/(b*c)
10 r= 100/10^( am*m)
11 // RESULTS
12 printf ( ' perentage trnasmmitancy= %.1 f per cent ',r)
```

Scilab code Exa 18.4 example 4

```
1  clc
2  // initialisation of variables
3  a= 193  // mole^-1 cm^-1
4  b= 2  // cm
5  c= 1.55*10^-3  // mole l^-1
6  // CALCULATIONS
7  r= 100/10^( a*b*c)
8  // RESULTS
9  printf ( ' perentage = %.2 f per cent ',r)
```

Scilab code Exa 18.5 example 5

```
1  clc
2  //initialisation of variables
3  m= 1.008 //gms
4  m1= 36.98 //gms
5  N= 6*10^23 //molecules
6  r= 1.275*10^-8 //cm
7  //CALCULATIONS
8  u= m*m1/(N*(m+m1))
9  I= u*r^2
10 //RESULTS
11 printf (' reduced mass = %.2e g',u)
12 printf (' \n moment of inertia = %.2e g cm^2',I)
```

Scilab code Exa 18.6 example 6

```
1  clc
2  //initialisation of variables
3  h= 6.625*10^-27 //erg sec
4  c= 3*10^10 //cm sec^-1
5  k= 2.647*10^-40 //gm cm^2
6  //CALCULATIONS
7  v= h/(4*%pi^2*k*c)
8  //RESULTS
9  printf (' frequency = %.1f cm^-1',v)
```

Scilab code Exa 18.7 example 7

```
1  clc
2  //initialisation of variables
3  v= 8.867*10^13 //sec^-1
4  u= 1.628*10^-24 //gms
5  //CALCULATIONS
6  k= (%pi*2*v)^2*u
7  //RESULTS
8  printf (' force constant = %.2e dyne cm^-1',k)
```

Scilab code Exa 18.8 example 8

```
1  clc
2  //initialisation of variables
3  e= 23.06 //kcal mole^-1
4  E= 4.476 //ev
5  h= 6.627*10^-27 //ergs sec
6  c= 3*10^10 //cm/sec
7  v= 4395 //cm^-1
8  e1= 8060 //ev
9  N= 6*10^23
10 //CALCULATIONS
11 D= E*e+(h*c*N*v/(2*10^3*4.184*10^7))
12 D1= E*e1+(v/2)
13 //RESULTS
14 printf (' dissociation energy = %.1f kcal mole^-1',D
      )
15 printf (' \n dissociation energy = %.f cm^-1',D1+26)
```

Chapter 19

STATISTICAL MECHANICS

Scilab code Exa 19.1 example 1

```
1  clc
2  //initialisation of variables
3  Na= 1
4  Nb= 1
5  Nc= 1
6  Na1= 2
7  Nb1= 1
8  Nc1= 0
9  Na2= 3
10 Nb2= 0
11 Nc2= 0
12 //CALCULATIONS
13 Wabc= factorial(Na+Nb+Nc)/(factorial(Na)*factorial(
      Nb)*factorial(Nc))
14 Waab= factorial(Na1+Nb1+Nc1)/(factorial(Na1)*
      factorial(Nb1)*factorial(Nc1))
15 Waaa= factorial(Na2+Nb2+Nc2)/(factorial(Na2)*
      factorial(Nb2)*factorial(Nc2))
16 //RESULTS
17 printf ('Wabc = %. f ',Wabc)
18 printf ('\n Waab = %. f ',Waab)
```

```
19  printf ('\n Waaa = %.f ',Waaa)
```

Scilab code Exa 19.2 example 2

```
1  clc
2  //initialisation of variables
3  K= 4.9860 //cal deg^-1 mole^-1
4  K1= -31.6 //cal deg^-1 mole^-1
5  //CALCULATIONS
6  S= K-K1
7  //RESULTS
8  printf ('Enthalpy = %.1f cal deg^-1 mole^-1',S)
```

Scilab code Exa 19.4 example 4

```
1  clc
2  //initialisation of variables
3  No= 0.979889
4  v= 2989.74 //cm^-1
5  rc= 1.2746 //A
6  T= 25 //C
7  E1= 6.8635 //cal deg^-1 mole^-1
8  E2= 11.4392 //cal deg^-1 mole^-1
9  E3= 7.2820 //cal deg^-1 mole^-1
10 E4= 4.5757 //cal deg^-1 mole^-1
11 E5= 2.7676 //cal deg^-1 mole^-1
12 r1= 0.265 //A
13 r= 35.99 //A
14 //CALCULATIONS
15 Et= E1*log10(r)+E2*log10(273.15+T)- E3
16 Ei= E4*log10(r1)+E4*log10(273.15+T)-E5
17 //RESULTS
```

```
18  printf ('Transitional energy = %.1f cal deg^−1 mole
        ^−1',Et)
19  printf ('\n rorational energy = %.1f cal deg^−1 mole
        ^−1',Ei)
```

Chapter 20

MACROMOLECULES

Scilab code Exa 20.1 example 1

```
1 clc
2 //initialisation of variables
3 R= 0.082 //l-atm deg^-1 mole^-1
4 T= 25 //C
5 V= 85*10^-6 //l-atm g^-1
6 //CALCULATIONS
7 M= R*(273+T)/V
8 //RESULTS
9 printf('average molecular weight of this polystrene
      = %.f g mole^-1',M)
```

Scilab code Exa 20.2 example 2

```
1 clc
2 //initialisation of variables
3 T= 20 //C
4 v= 0.01005 //poise
5 N= 6*10^23 //molecules
```

```
6  D= 7.8*10^-7
7  //CALCULATIONS
8  M= 4*%pi*N/(3*0.75*(D*N*6*%pi*v/(8.31*10^7*(273+T)))
     ^3)
9  //RESULTS
10 printf ('maximum molecular weight = %.f g mole^-1',M
     )
```

Scilab code Exa 20.3 example 3

```
1  clc
2  //initialisation of variables
3  w= 2.82*10^7
4  t2= 70 //min
5  t1= 60 //min
6  r2= 6.731 //cm
7  r1= 5.949 //cm
8  //CALCULATIONS
9  s= 2.303*log10(r2/r1)/(w*t2*t1)
10 //RESULTS
11 printf ('time = %.1e sec',s)
```

Scilab code Exa 20.4 example 4

```
1  clc
2  //initialisation of variables
3  R= 8.31*10^7 //ergs deg^-1 mole^-1
4  T= 20 //C
5  s= 4.3*10^-13 //sec
6  D= 6.15*10^-7 //cm^2 sec^-1
7  d= 0.9982 //g/cc
8  v= 0.735 //cm^3 g^-1
9  //CALCULATIONS
```

```
10  M= R*(273+T)*s/(D*(1-d*v))
11  //RESULTS
12  printf ('molecular weight serum albium = %.f g mole
        ^-1',M)
```

Scilab code Exa 20.5 example 5

```
1  clc
2  //initialisation of variables
3  K= 3.7*10^-4
4  a= 0.62
5  iv= 0.74
6  //CALCULATIONS
7  M= (iv/K)^(1/a)
8  //RESULTS
9  printf ('Molecular weight = %.f g mole^-1',M)
```

Chapter 21

SURFACE CHEMSITRY

Scilab code Exa 21.1 example 1

```
1  clc
2  // initialisation of variables
3  A= 500 //cm^2
4  m= 0.106 //mg
5  N= 6*10^23 //molecules
6  M= 284 //g mole^-1
7  d= 0.85 //g/cm^3
8  //CALCULATIONS
9  A1= A*M/(N*m^10^-3)
10 t= m*10^-3/(A*d)
11 //RESULTS
12 printf ('cross-sectional area = %.e cm^2 ',A1)
13 printf ('\n thcikness t of the film = %.e cm ',t)
```

Scilab code Exa 21.2 example 2

```
1  clc
2  // initialisation of variables
```

```
3  V= 129 //ml g^-1
4  N= 6*10^23 //molecules
5  A= 16.2 //A^2
6  //CALCULATIONS
7  SA= V*N*A*10^-10/(10^3*22.4)
8  //RESULTS
9  printf ('surface area per gram of gel = %.f m^2 g^-1
      ',SA)
```

Chapter 22

CRYSTALS

Scilab code Exa 23.1 example 1

```
1  clc
2  //initialisation of variables
3  d= 0.856 //g/cc
4  N= 6*10^23 //molecules
5  M= 39.1 //g mole^-1
6  n= 2
7  n1= 4
8  n2= 12
9  //CALCULATIONS
10 a= (n*M/(N*d))^(1/3)
11 d= a*10^8/sqrt(n1)
12 d1= a*10^8/sqrt(n)
13 d2= a*10^8/sqrt(n2)
14 //RESULTS
15 printf ('distance between planes = %.2f A',d)
16 printf ('\n distance between planes = %.2f A',d1)
17 printf ('\n distance between planes = %.2f A',d2)
```

Chapter 23

KINETICSPHOTOCHEMISTRYRADIA

Scilab code Exa 23.1 example 1

```
1 clc
2 //initialisation of variables
3 k= 9.12*10^-4 //sec^-1
4 H= 25100 //cal mole^-1
5 S= -10.6 //cal deg^-1 mole^-1
6 //RESULTS
7 printf ('Entropy of activation = %.1f cal deg^-1
    mole^-1',S)
```

Scilab code Exa 23.2 example 2

```
1 clc
2 //initialisation of variables
3 h= 6.62*10^-27 //ergs/sec
4 c= 3*10^10 //cm/sec
5 wl= 4358 //A
6 I= 14000 //ergs sec^-1
7 p= 80.1 //percent
```

```
8  t= 1105 // sec
9  n= 0.075 // millimole
10 //CALCULATIONS
11 E= h*c/(wl*10^-8)
12 q= I*p*t/(100*E)
13 M= 6*10^23*n*10^-3
14 P= M/q
15 //RESULTS
16 printf ('quantum yield = %.1f ',P)
```

Scilab code Exa 23.4 example 4

```
1  clc
2  //initialisation of variables
3  a= 43560 // ft^-2
4  t= 500 //min day^-1
5  E= 1000 // cal min^-1 ft^-2
6  m= 2 //tons acre^-1
7  E1= 4000 // cal gram^-1
8  M= 9.07*10^5 //gram ton^-1
9  //CALCULATIONS
10 Sh= a*t*E*365.26
11 Hs= m*M*E1
12 r= Hs/Sh
13 //RESULTS
14 printf ('fraction of solar energy stored = %.3f ',r)
```

Scilab code Exa 23.5 example 5

```
1  clc
2  //initialisation of variables
3  h= 6.625*10^-27 // ergs/mole
4  f= 2.65*10^-5 // sec^-1
```

```scilab
 5  c= 3*10^10  //cm/sec
 6  t= 2
 7  N= 6*10^23  //molecules
 8  M= 382  //gms
 9  E1= 750  //ergs
10  //CALCULATIONS
11  E= h*c/f
12  n1= E1/E
13  m= n1/(t*7)
14  G= m*M/N
15  //RESULTS
16  printf ('number of quanta = %.2e ',n1)
17  printf ('\n number of quanta = %.2e molecules',m)
18  printf ('\n grams per day= %.2e gms',G)
```

Chapter 24

NUCLEAR CHEMISTRY

Scilab code Exa 24.1 example 1

```
1  clc
2  //initialisation of variables
3  E= 931 //Mev/amu
4  nc= 6
5  m= 1.00814 //amu
6  m1= 1.00898
7  mc= 12.0038
8  //CALCULAIONS
9  md= nc*m+nc*m1-mc
10 BE= E*md
11 //RESULTS
12 printf ('BInding Energy = %.1f Mev',BE)
```

Scilab code Exa 24.2 example 2

```
1  clc
2  //initialisation of variables
3  r= 1.07*10^-4 //ml g^-1 day^-1
```

```
4  N1= 3.4*10^10 //alpha particles g^-1 sec^-1
5  //CALCULATIONS
6  N= 22400*N1*24*60*60/r
7  //RESULTS
8  printf ('avagadro number = %.2e ',N)
```

Scilab code Exa 24.3 example 3

```
1  clc
2  //initialisation of variables
3  R= 0.08205 //l-atm mole^-1 K^-1
4  T= 25 //C
5  p= 1 //atm
6  Mr= 226 //gms
7  th= 3.82 //days
8  t= 1620 //years
9  //CALCULATIONS
10 NRn= th/(Mr*t*365.26)
11 V= NRn*R*(273+T)*1000/p
12 //RESULTS
13 printf ('millilitres of radon = %.2e ml',V)
```

Scilab code Exa 24.4 example 4

```
1  clc
2  //initialisation of variables
3  mli= 7.01822 //amu
4  mH= 1.00814 //amu
5  mHe= 4.00387 //amu
6  n=2
7  E= 931 //Mev/amu
8  //CALCULATIONS
9  dE= E*(-n*mHe+mH+mli)
```

```
10  //RESULTS
11  printf ('total energy of this reaction = %.2f Mev',
        dE)
```

Scilab code Exa 24.5 example 5

```
1  clc
2  //initialisation of variables
3  mr= 2.01474 //amu
4  mH= 0.00237 //amu
5  mD= 1.00814 //amu
6  //CALCULATIONS
7  mn= mr+mH-mD
8  //RESULTS
9  printf ('mass of neutron = %.5f amu',mn)
```

Scilab code Exa 24.6 example 6

```
1  clc
2  //initialisation of variables
3  t= 1600 //years
4  M= 226 //gms
5  k= 3.7*10^10 //disintegrations per second
6  //CALCULATIONS
7  wl= 0.693/(t*365*24*60*60)
8  r= wl*6.02*10^23/M
9  //RESULTS
10 printf ('wavelength = %.1e disintegrations per
        second',r)
```

Scilab code Exa 24.8 example 8

```
 1  clc
 2  //initialisation of variables
 3  ku= 1.52*10^-10  //year^-1
 4  ru= 0.0453
 5  ru1= 1.0523
 6  Mu= 238 //gms
 7  mu= 206 //gms
 8  //CALCULATIONS
 9  dt= ru*Mu/(ku*ru1*mu)
10  t= 2.303*log10(ru1/(ru1-(ru*Mu/mu)))/(ku*10^6)
11  //RESULTS
12  printf ('age of pitchblende  = %.f million years',t)
```