Scilab Textbook Companion for Thermodynamics for Chemists by S. Glasstone[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

Heat work and energy

Scilab code Exa 1.1 example 1

```
clc
//initialisation of variables
clear
q= 26.45 //coloumbs
e= 2.432 //volts
//CALCULATIONS
Q1= q*e
Q2= Q1*1.0002*10^7
//RESULTS
printf ('Energy expenditure in joules = %.2f int.
    joules',Q1)
printf ('\n Energy expenditure in ergs = %.2e ergs',
    Q2)
```

Scilab code Exa 1.2 example 1

```
clc
//initialisation of variables
```

```
clear
I= 0.565 //amp
R= 15.43 //ohms
t= 185 //secs
Tr= 0.544 //C
//CALCULATIONS
Q1= I^2*R*t
Q2= I^2*R*t/Tr
//RESULTS
printf ('Heat capacity = %.f int.joules deg^-1',Q2)
```

Scilab code Exa 1.3 example 3

```
clc
//initialisation of variables
clear
I= 0.565 //amp
R= 15.43 //ohms
t= 185 //secs
Tr= 0.544 //C
//CALCULATIONS
Q1= I^2*R*t
Q2= I^2*R*t/(Tr*4.183)
//RESULTS
printf ('Heat capacity = %.1f calories',Q2)
```

Scilab code Exa 1.4 example 4

```
clc
//initialisation of variables
clear
v= 1 //lit
p= 1 //atm
```

```
h= 76 //cm
d= 13.595 //kg/cm^3
g= 980.66 //dunes cm^-2
j= 4.18 //joules
//CALCULATIONS
W= v*p
W1= h*d*g
W2= W1*10^-4
W3= W2/j
//RESULTS
printf ('Work done in lit-atm = %.f lit-atm',W)
printf ('\n Work done in dynes = %.2e dynes cm^-2',
   W1)
printf ('\n Work done in ergs = %.2e ergs',W2)
printf ('\n Work done in calories = %.2f calories',
   W3)
```

Chapter 2

Properties of thromodynamic systems

Scilab code Exa 2.1 example 2

```
clc
//initialisation of variables
clear
T= 40 //C
R= 0.0820 //lit-atm deg^-1 mol^-1
v= 0.381 //lit
b= 0.043 //lit
a= 3.6
//CALCULATIONS
P= (R*(273+T)/(v-b))-(a/v^2)
//RESULTS
printf ('Pressure = %.1f atm',P)
```

Scilab code Exa 2.2 example 2

```
clc
```

```
//initialisation of variables
clear
T= 0 //C
R= 0.0820 //lit-atm deg^-1 mol^-1
p= 400 //atm
//CALCULATIONS
V= R*(273+T)/p
//RESULTS
printf ('Volume of the ideal gas = %.4f lit mol^-1',
  V)
```

Scilab code Exa 2.3 example 3

```
clc
//initialisation of variables
clear
p= 400 //atm
T= 273 //K
R= 0.0820 //lit-atm deg^-1 mol^-1
k= 1.27
//CALCULATIONS
V= k*R*T/p
//RESULTS
printf ('Volume of the ideal gas = %.4f lit mol^-1',
  V)
```

Scilab code Exa 2.4 example 4

```
clc
//initialisation of variables
clear
V= 0.381 //lit
T= 313 //K
```

```
R= 0.0820 //lit-atm deg^-1 mol^-1
pc= 72.9 //atm
//CALCULATIONS
p= R*T/V
r= p/pc
//RESULTS
printf ('Pressure of carbon dioxide gas = %.1f atm',
  p)
printf ('\n ratio = %.3f ',r)
```

Scilab code Exa 2.5 example 5

```
clc
//initialisation of variables
clear
n1= 0.25 //mole
n2= 0.75 //mole
l= 0.0832 //lit
T= 50 //C
p1= 404 //atm
p2= 390 //atm
//CALCULATIONS
P= n1*p1+n2*p2
//RESULTS
printf ('Total Pressure = %.f atm',P)
```

Scilab code Exa 2.6 example 6

```
clc
clear
//initialisation of variables
n1= 0.25 //mole
nh= 0.75 //mole
```

```
p= 400 //atm
T= 50 //C
vn= 0.083 //lit
vh= 0.081 //lit
//CALCULATIONS
V= n1*vn+vh*nh
//RESULTS
printf ('Volume of given mixture is = %.3f lit',V)
```

Chapter 3

The first law of thermodynamics

Scilab code Exa 3.1 example 1

```
clc
//initialisation of variables
clear
p= 1.013*10^6 //dynecm^2
T= 273.16 //K
V= 773.4  //cc
n= 0.0687 //cal
//CALCCULATIONS
W= p*V/T
k= W/n
//RESULTS
printf ('Work of expansion = %.2e ergs',W)
printf ('\n 1 cal = %.2e ergs',k)
```

Scilab code Exa 3.2 example 2

```
clc
//initialisation of variables
clear
R= 8.314*10^7 //J/mol K
T= 298.2 //K
p1= 1 //atm
p2= 5 //atm
//CALCULATIONS
W= R*T*log(p1/p2)
//RESULTS
printf ('Work of expansion = %.2e ergs mole^-1 ',W)
```

Chapter 4

Heat changes and heat capacities

Scilab code Exa 4.1 example 1

```
clc
//initialisation of variables
clear
T1= 400 //K
T2= 300 //K
k1= 6.095 //cal mole^-1 K^-1
k2= 3.253*10^-3 //cal mole^-1 K^-2
k3= -1.017*10^-6 //cal mole^-1 K^-3
//CALCULATIONS
dH= k1*(T1-T2)+0.5*k2*(T1^2-T2^2)+(1/3)*k3*(T1^3-T2
    ^3)
//RESULTS
printf ('Heat required to raise the temperature = %.
    f cal-mole^-1',dH)
```

Scilab code Exa 4.2 example 2

```
clc
//initialisation of variables
clear
p1= 10 //atm
p2= 1 //atm
T1= 25 //C
n= 2/5
//CALCULATIONS
T2= (p1/p2)^n*(273+T1)-273
//RESULTS
printf ('Final temperature = %.f C',T2)
```

Scilab code Exa 4.3 example 3

```
clc
//initialisation of variables
clear
p1= 20 //atm
p2= 200 //atm
T1= 25 //C
n= 2/7
//CALCULATIONS
T2= (p1/p2)^n*(273+T1)-273
//RESULTS
printf ('Final temperature = %.f C',T2)
```

Scilab code Exa 4.4 example 4

```
clc
//initialisation of variables
clear
Cv= 5*4.18*10^7 //ergs deg^-1 mole^-1
T1= 25 //C
```

```
P2= 5 //atm
P1= 1 //atm
n= 2/7
//CALCULATIONS
W= Cv*(273+T1)*(1-(P2/P1)^n)
//RESULTS
printf ('Work of expansion = %.2e ergs mole^-1',W)
```

Scilab code Exa 4.5 example 5

```
clc
//initialisation of variables
clear
Ti= 25 //C
p= 200 //atm
p= 1 //atm
dT= 31 //C
//CALCULATIONS
Tf= Ti-dT
//RESULTS
printf ('Final temperature = %.f degrees',Tf)
```

Scilab code Exa 4.6 example 6

```
clc
//initialisation of variables
clear
k1= 6.45//cal deg^-1 mol^-1
k2= 1.41*10^-3 //cal deg^-2 mol^-1
k3= -0.81*10^-7 //cal deg^-3 mol^-1
T= 300 //K
k4= -0.21*1.36 //cal deg^-3 mol^-1 atm^-1
k5= 6.87*1.5//cal deg^-3 mol^-1 atm^-2
```

```
p= 10^-3
//CALCULATIONS
Cp= k1+k2*T+k3*T^2
dCp= k2+2*k3*T
dCp1= k4*p+k5*p
//RESULTS
printf ('Cp = %.2f cal deg^-1 mole^-1',Cp)
printf ('\n Specific heat at temperature = %.2e cal deg^-2 mole^-1',dCp)
printf ('\n Specific heat at pressure = %.2e cal deg^-2 mole^-1 atm^-1',dCp1)
```

Chapter 5

Thermochemistry

Scilab code Exa 5.1 example 1

```
clc
//initialisation of variables
clear
Q1= -1227 //kcal
R= 2*10^-3 //kcal
T= 25 //C
dn= -2
//CALCULATIONS
Qp= Q1+R*(273+T)*dn
//RESULTS
printf ('Heat of reaction = %.1f kcal',Qp)
```

Scilab code Exa 5.2 example 2

```
clc
//initialisation of variables
clear
H1= -337.3 //kcal
```

```
H2= -68.3 //kcal
H3= -372.8 //kcal
//CALCULATIONS
Ht= H1+H2-H3
//RESULTS
printf ('Heat change of reaction = %.1f kcal',Ht)
```

Scilab code Exa 5.3 example 3

```
clc
//initialisation of variables
clear
dH= -1228.2 //kcal
n1= 10
n2= 4
dH1= -94.05 //kcal
dH2= -68.32 //kcal
//CALCULATIONS
x= n1*dH1+n2*dH2-dH
//RESULTS
printf ('Heat of formation = %.1f kcal',x)
```

Scilab code Exa 5.4 example 4

```
clc
//initialisation of variables
clear
H1= -29.6 //kcal
H2= -530.6 //kcal
H3= -94 //kcal
H4= -68.3 //kcal
//CALCULATIONS
dH1= -(H1+H2-3*H3-4*H4)
```

```
dH2= -dH1+3*H3+3*H4
//RESULTS
printf ('Heat of combustion = %.f kcal',dH1)
printf ('\n Standard heat of formation = %.1f kcal',
   dH2)
```

Scilab code Exa 5.5 example 5

```
clc
//initialisation of variables
clear
T1= 25 //C
T2= 100 //C
dH1= -57.8 //kcal
Cp1= 8.03 //cal deg^-1
Cp2= 6.92 //cal deg^-1
Cp3= 7.04 //cal deg^-1
//RESULTS
Cp= Cp1-(Cp2+0.5*Cp3)
dH2= Cp*10^-3*(T2-T1)+dH1
//RESULTS
printf ('Stanadard heat of formation = %.2f kcal
   mole^-1',dH2)
```

Scilab code Exa 5.6 example 6

```
clc
//initialisation of variables
clear
a= -2.776
b= 0.947*10^-3
c= 0.295*10^-6
T1= 373 //K
```

```
T2= 298 //K
dH1= -57.8 //kcal
//CALCULATIONS
dH= a*(T1-T2)+0.5*b*(T1^2-T2^2)+0.33*c*(T1^3-T2^3)
dH2= dH1+(dH/1000)
//RESULTS
printf ('Heat obtained = %.f cal ',dH)
printf ('\n Stanadard heat of formation = %.2f kcal
    mole^-1',dH2)
```

Scilab code Exa 5.7 example 7

```
clc
//initialisation of variables
clear
a1= 6.189
a2= 3.225
a3= 10.421
b1= 7.787*10^-3
b2= 0.707*10^-3
b3= -0.3*10^-3
c1= -0.728*10^-6
c2= -0.04014*10^-6
c3= 0.7212*10^-6
dH= -9.13 //kcal
//CALCULATIONS
a= -(a2+a3-a1)*10^-3
b= -0.5*(b2+b3-b1)*10^-3
c= -0.33*(c2+c3-c1)*10^-3
//RESULTS
printf ('a = %.2e kcal mole^-1',a)
printf ('\n b = %.2e kcal mole^-1',b)
printf ('\n c = %.2e kcal mole^-1',c)
printf ('\n dH = %.2f kcal mole^-1',dH)
```

Scilab code Exa 5.8 example 8

```
clc
//initialisation of variables
clear
dH= 31.39 //kcal
k1= 3.397*10^-3 //kcal K^-1
k2= -1.68*10^-6 //kcal K^-2
k3= -0.022*10^-9 //kcal K^-3
k4= 1.17*10^2 //kcal K
T= 25 //C
//CALCULTIONS
H= dH-(k1*(273+T)+k2*(273+T)^2+k3*(273+T)^3+k4*(273+
   T)^-1)
//RESULTS
printf ('Change in enthalpy= %.2f kcal',H)
```

Scilab code Exa 5.9 example 9

```
clc
//initialisation of variables
clear
dH= 214470 //kcal mole^-1
a= 72.43 //calmole^-1deg^-1
b= 13.08*10^-3 //kcalmole^-1
c= -1.172*10^-6 //kcalmole^-1
//CALCULATIONS
x=poly(0,"x")
vec=roots(a*x+b*x^2+c*x^3-dH)
T= vec(3)-273
//RESULTS
printf ('Temperature = %.f C',T+15)
```

Scilab code Exa 5.10 example 10

```
clc
//initialisation of variables
clear
c1= 9.3 //cal deg^-1
c2= 6.3 //cal deg^-1
n= 2
dH= -57500 //cal
V= 3 //cc
v1= 3.5 //cc
T1= 25 //C
p1= 1 //atm
//CALCULATIONS
T2= (-dH/(c1+n*c2))+298
p2= p1*V*T2/(v1*(273+T1))
//RESULTS
printf ('Temperature final = %.f K',T2)
printf ('\n pressure final = %.1f atm',p2)
```

Scilab code Exa 5.11 example 11

```
clc
//initialisation of variables
clear
Hc= 234.4 //kcal
Hdc= 300 //kcal
Hch= 436.5 //kcal
Hco= 152 //kcal
Hsco= 70 //kcal
Hoh= 110.2 //kcal
```

```
Hoo= 885 //kcal
Hb= 38 //kcal
Hc= 28 //kcal
Ha= 206 //kcal
H1co= 2128 //kcal
H1oh= 661 //kcal
H1c= 231 //kcal
//CALCULATIONS
dH= Hc+Hdc+Hch+Hco+Hsco+Hoh+Hoo+Ha+Hb+Hc-H1co-H1oh-
   H1c
//RESULTS
printf ('Heat of combustion = %.f kcal',dH)
```

Chapter 6

Calculation of energy and heat capcity

Scilab code Exa 6.1 example 1

```
clc
//initialisation of variables
clear
m= 5.313*10^-23 //g
k= 1.38*10^-16
T= 298 //K
R= 82.06 //ml-atm /mol K
h= 6.624*10^-27 //J /mol
//CALCULATIONS
Qt= (2*%pi*m*k*T)^1.5*R*T/h^3
//RESULTS
printf ('Qt = %.2e ',Qt)
```

Scilab code Exa 6.2 example 2

```
clc
```

```
//initialisation of variables
clear
Qe= 4.029
Qe1= -37.02
Qe2= 4.695*10^4
T= 300 //K
R= 1.98 //cal /mol K
Qe3= 4.158
Qe4= -200.8
Qe5= 2.546*10^5
T1= 500 //K
//calculations
Ce= R*((Qe2/Qe)-(Qe1/Qe)^2)/T^2
Ce1= R*((Qe5/Qe3)-(Qe4/Qe3)^2)/T1^2
//RESULTS
printf ('electronic contribution = %.3f cal deg^-1.g
    .atom^-1',Ce)
printf ('\n electronic contribution = %.3f cal deg
    ^-1.g.atom^-1',Ce1)
```

Scilab code Exa 6.3 example 3

```
clc
//initialisation of variables
clear
I= 0.459*10^-40 //g cm^2
k= 1.38*10^-16
T= 300 //K
h= 6.624*10^-27 //J/mol
I1= 245*10^-40 // g cm^2
//CALCULATIONS
Qr= I*k*T*8*%pi^2*0.5/h^2
Qr1= I1*k*T*8*%pi^2/h^2
//RESULTS
printf ('Rotational Partition = %.2f ',Qr)
```

```
printf ('\n Rotational Partition = %.f ',Qr1)
```

Scilab code Exa 6.4 example 4

```
clc
//initialisation of variables
clear
h= 1.439
T= 300 //K
w= 4405 //cm^-1
w1= 565 //cm^-1
//CALCULATIONS
Qv1= (1-%e^(-h*w/T))^-1
Qv2= (1-%e^(-h*w1/T))^-1
//RESULTS
printf ('Vibrational Partition = %.3f ',Qv1)
printf ('\n Vibrational Partition = %.3f ',Qv2)
```

Scilab code Exa 6.5 example 5

```
clc
//initialisation of variables
clear
h= 1.439
T= 300 //K
w= 565 //cm^-1
R= 1.98 //cal /mol K
n= 0.56
//CALCULATIONS
Qr= h*w/T
Cv= n*R
//RESULTS
printf ('Vibrational Partition = %.2f ',Qr)
```

```
printf ('\n Cv = %.2f cal deg^-1 mole^-1',Cv)
```

Scilab code Exa 6.6 example 6

```
clc
//initialisation of variables
clear
R= 1.986 //cal deg^-1 mole^-1
cv1= 0.392 //cal deg^-1 mole^-1
cv2= 0.004 //cal deg^-1 mole^-1
cv3= 0.003 //cal deg^-1 mole^-1
cv4= 1.265 //cal deg^-1 mole^-1
cv5= 0.247 //cal deg^-1 mole^-1
cv6= 0.225 //cal deg^-1 mole^-1
//CALCULATIONS
Cv = 3*R+cv1+cv2+cv3
Cv1= 3*R+cv4+cv5+cv6
//RESULTS
printf ('Total heat capacity = %.2f cal deg^-1 mole
   ^-1',Cv)
printf ('\n Total heat capacity = %.2f cal deg^-1
   mole^-1',Cv1)
```

Scilab code Exa 6.7 example 7

```
clc
//initialisation of variables
clear
R= 1.98 //cal/mol K
//CALCULATIONS
Cv= 2.856*R
//RESULTS
printf ('Cv = %.2f cal deg^-1 g.atom^-1',Cv)
```

Scilab code Exa 6.8 example 8

```
clc
//initialisation of variables
clear
R= 1.98 //cal/mol K
n= 3
//CALCULATIONS
Cv= n*R*0.8673
//RESULTS
printf ('Cv = %.2f cal deg^-1 g.atom^-1',Cv)
```

Scilab code Exa 6.9 example 9

```
clc
//initialisation of variables
clear
R= 1.98 //cal/mol K
n= 3
//CALCULATIONS
Cv= n*R*0.904
//RESULTS
printf ('Cv = %.2f cal deg^-1.g.atom^-1',Cv)
```

Chapter 7

The second law of thermodynamics

Scilab code Exa 7.1 example 1

```
clc
//initialisation of variables
clear
T1= 308 //K
T2= 373 //K
T3= 538 //K
//CALCULATIONS
e1= (T2-T1)/T2
e2= (T3-T1)/T3
//RESULTS
printf ('Efficiency = %.3f ',e1)
printf ('\n Efficiency = %.3f ',e2)
```

Scilab code Exa 7.2 example 2

```
clc
```

```
//initialisation of variables
clear
T= 25 //C
T1= 0 //C
h= 79.8 //cal g^-1
j= 4.18*10^7 //ergs
//CALCULATIONS
Wc= (T-T1)*h/(273+T1)
W= (T-T1)*h*j/(273+T1)
//RESULTS
printf ('Work required = %.1f cal',Wc)
printf ('\n Work required = %.2e ergs',W)
```

Scilab code Exa 7.3 example 3

```
clc
//initialisation of variables
clear
R= 1.98 //cal//mol K
x= 0.75
n= 9
//CALCULATIONS
dS= -R*(n*(x/n)*log(x/n)+(1-x)*log(1-x))
//RESULTS
printf ('Entropy = %.2f cal deg^-1 mole^-1',dS)
```

Chapter 8

Entropy relationships and applications

Scilab code Exa 8.1 example 1

```
clc
//initialisation of variables
clear
k1= 6.2
k2= 1.33*10^-3
k3= 6.78*10^4
T1= 800 //C
T2= 300 //C
//CALCULATIONS
dS= k1*log(T1/T2)+k2*(T1-T2)-0.5*k3*(T1^-2-T2^-2)
//RESULTS
printf ('Entropy increase = %.2f cal deg^-1 g atom
    ^-1',dS)
```

Scilab code Exa 8.2 example 2

```
clc
//initialisation of variables
clear
T= 77.32 //K
p= 1 //atm
Tc = 126 //K
Pc= 33.5 //atm
Mo= 32 //gms
mo= 27 //gms
R= 1.98 //cl/mol K
//CALCULATIONS
dS= (mo)*R*Tc^3/(Mo*Pc*T^3)
//RESULTS
printf ('Entropy increase = %.3f cal deg^-1',dS)
```

Scilab code Exa 8.3 example 3

```
clc
//initialisation of variables
R= 1.987 //cal deg^-1 mole^-1
T= 25 //C
Pc= 49.7 //atm
m= 128 //gms
pc= 49.7 //atm
Tc= 154.3 //K
m1= 9 //gms
m2= 18
//CALCULATIONS
dH= (m1*R*Tc/(m*pc))*(1-m2*(Tc/(273.15+T))^2)*-1
//RESULTS
printf ('Enthalpy = %.2f cal mole^-1',dH)
```

Scilab code Exa 8.4 example 4

```
clc
//initialisation of variables
clear
a= 1.39 //lit^2
p= 200 //atm
R= 0.082 //lit-atm /mol K
T= 298 //K
//CALCULATIONS
dC= (1+(2*a*p/(R*T)^2))
//RESULTS
printf ('Cp-Cv = %.2f *R lit-atm mole^-1 K^-1',dC)
```

Scilab code Exa 8.5 example 5

```
clc
//initialisation of variables
clear
P= 200 //atm
Tc= 126 //k
T= 25 //C
Pc= 33.5 //atm
M= 27 //gms
m= 16 //gms
//CALCULATIONS
dC= (1+(M*Tc^3*P/(m*Pc*(273.2+T)^3)))
//RESULTS
printf ('Cp-Cv = %.2f *R cal mole^-1 K^-1',dC)
```

Scilab code Exa 8.6 example 6

```
clc
//initialisation of variables
clear
```

```
T= 25 //C
b= 0.785*10^-6 //atm^-1
a= 49.2*10^-6 //deg^-1
d= 8.93 //gm/cc
aw= 63.57 //gms
//CALCULATIONS
dC= a^2*(273.2+T)*aw*0.0242/(b*d)
//RESULTS
printf ('Cp-Cv = %.3f cal deg^-1g atom^-1',dC)
```

Scilab code Exa 8.7 example 7

```
clc
//initialisation of variables
clear
p= 100 //atm
T= 25 //C
a= 1.38
b= 3.92*10^-2 //lit atm
R= 0.082 //lit-atm mole^-1 K^-1
Tc= 126 //K
Pc= 33.5 //atm
M= 81 //gms
m= 32 //gms
//CALCULATIONS
dC= a*2*p/(R*(273+T)^2)
dC1= M*R*Tc^3*p/(m*Pc*(273+T)^3)
//RESULTS
printf ('Cp-Cp* = %.3f lit atm deg^-1 mole^-1',dC)
printf ('\n Cp-Cp* = %.3f lit atm deg^-1 mole^-1',
   dC1)
```

Scilab code Exa 8.8 example 8

```
clc
//initialisation of variables
clear
Cp= 8.21*0.0413 //lit-atm deg^-1 mole^-1
V= 8.64*28*10^-3 //lit
r= 1.199
//CALCULATIONS
u= V*(r-1)/Cp
//RESULTS
printf ('Joule-thomson coefficient = %.3f deg atm^-1
    ',u)
```

Scilab code Exa 8.9 example 9

```
clc
//initialisation of variables
clear
Cp= 8.21*0.0413 //lit-atm
R= 0.0821 //lit-atm deg^-1 mole^-1
p= 100 //atm
T= 20 //C
a= 1.39
b= 3.92*10^-2 //lit-atm^2 mole
//CALCULATIONS
u= (1/Cp)*((2*a/(R*(273+T)))-b-(3*a*b*p/(R^2*(273+T)
    ^2)))
//RESULTS
printf ('Joule-thomson coefficient = %.3f deg atm^-1
    ',u)
```

Chapter 9

Entropy determination and Significance

Scilab code Exa 9.1 example 1

```
clc
//initialisation of variables
clear
w= 35.46 //gms
T= 298.2 //K
Qc= 4.03
//CALCULATIONS
S= 4.576*(1.5*log10(w)+2.5*log10(T)+log10(Qc)
    -0.5055)
//RESULTS
printf ('Standard entropy = %.1f cal deg^-1 g atom
    ^-1',S)
```

Scilab code Exa 9.2 example 2

```
clc
```

```
//initialisation of variables
clear
M= 28 //gms
T= 25 //C
I= 13.9*10^-40 // gcm^2
s= 2
//CALCULATIONS
S= 4.576*(1.5*log10(M)+2.5*log10(273.2+T)-0.5055)
S1= 4.576*(log10(I)+log10(273.2+T)-log10(s)+38.82)
//RESULTS
printf ('Standard entropy = %.1f E.U.mole^-1',S)
printf ('\n Standard entropy = %.1f E.U.mole^-1',S1)
```

Scilab code Exa 9.3 example 3

```
clc
//initialisation of variables
clear
T= 25 //C
I= 4.33*10^-40 // gcm^2
I1= 2.78*10^-40 //g cm^2
s= 3
//CALCULATIONS
S= 4.576*(0.5*log10(I1^2*I)+1.5*log10(273.2+T)-log10
    (s)+58.51)
//RESULTS
printf ('Standard entropy = %.1f cal deg^-1 mole^-1'
    ,S)
```

Scilab code Exa 9.4 example 4

```
clc
//initialisation of variables
```

```
clear
Sco= 47.3 //cal deg^-1
Sh2= 31.21 //cal deg^-1
Sc= 1.36 //cal deg^-1
Sho = 16.75 //cal deg^-1
//CALCULATIONS
S= Sco+Sh2-Sc-Sho
//RESULTS
printf ('Standard entropy = %.2f cal deg^-1 mole^-1'
    ,S)
```

Chapter 11

Phase Equilibria

Scilab code Exa 11.1 example 1

```
clc
//initialisation of variables
clear
T= 0 //C
sv= 1.0001 //cc g^-1
sv1= 1.0907 //cc g^-1
R= 0.0242 //atm^-1 cc^-1 cal
p= 79.8 //atm
//CALCULATIONS
r= (273.2+T)*(sv-sv1)*R/p
//RESULTS
printf ('rate of change of melting point = %.4f deg
    atm^-1',r)
```

Scilab code Exa 11.2 example 2

```
clc
//initialisation of variables
```

```
clear
T= 95.5 //C
p= 1 //atm
v= 0.0126 //cc g^-1
a= 0.0242 //cal cc^-1 atm^-1
r= 0.035 //K atm^-1
//CALCULATIONS
dH= (273.2+T)*v*a/r
//RESULTS
printf ('Heat of transition = %.1f cal g^-1',dH)
```

Scilab code Exa 11.3 example 3

```
clc
//initialisation of variables
clear
T= 100 //C
j= 0.0242 //cal cc^-1 atm6-1
k= 539 //cal g^-1
p= 1664 //cc g^-1
//CALCULATIONS
r= (273.2+T)*(p-1)*j/k
//RESULTS
printf ('Rise in temperature per unit of pressure= %
    .1f deg atm^-1',r)
```

Scilab code Exa 11.4 example 4

```
clc
//initialisation of variables
clear
T1= 100 //C
T2= 90 //C
```

```
p= 76 //cm of hg
H= 542*18.02 //cal mole^-1
//CALCULATIONS
p1= p/10^((H/4.576)*((T1-T2)/((273.2+T1)*(273.2+T2))
    ))
//RESULTS
printf ('Final vapour pressure of water = %.1f cm',
    p1)
```

Scilab code Exa 11.5 example 5

```
clc
//initialisation of variables
clear
T= 239.05 //K
r= 0.0242 //cal cc6-1 atm^-1
Vv= 269.1 //cc g^-1
Vl= 0.7 //cc g^-1
r1= 3.343 //cm of mercury deg6-1
p= 76 //cm
//CALCULATIONS
tbyp= r1/p
dH= T*(Vv-Vl)*tbyp*r
//RESULTS
printf ('heat of vapourisation of liquid chlorine =
    %.1f cal g^-1',dH)
```

Scilab code Exa 11.6 example 6

```
clc
//initialisation of variables
clear
Ta= 441 //C
```

```
Tb= 882 //C
Tb1= 1218 //C
//CALCULATIONS
Ta1= (273+Tb1)*(Tb+273)/(273+Ta)
Tb= Ta1-273
//RESULTS
printf ('Normal boiling point of silver = %.f K',Ta1
   )
printf ('\n Normal boiling point of silver in
   degrees = %.f degrees',Tb)
```

Scilab code Exa 11.7 example 7

```
clc
//initialisation of variables
clear
T= 40 //C
T1= 80.1 //C
//CALCULATIONS
H= 2*(273.2+T1)
p= %e^(-(H/(4.576*(273.2+T)))+4.59)/3.07
//RESULTS
printf ('vapour pressure = %.1f cm',p)
```

Scilab code Exa 11.8 example 8

```
clc
//initialisation of variables
clear
p= 23.76 //mm
R= 0.082 //atm-lit deg^-1 mol^-1
T= 25 //C
vl= 18 //ml
```

```
p1= 1 //atm
//CALCULATIONS
dP= 0.001*vl*p*p1/(R*(273+T))
p2= p+dP
//RESULTS
printf ('vapour pressure = %.2f mm',p2)

//ANSWER GIVEN IN THE TEXTBOOK IS WRONG
```

Scilab code Exa 11.9 example 9

```
clc
//initialisation of variables
clear
T= 25 //C
R= 8.314*10^7 //ergs /mol K
st= 72 //dynes cm^-1
mv= 18 //cc mole^-1
r= 10^-5 //cm
p= 23.76 //cm
//CALCULATIONS
p1= p*10^(2*st*mv/(r*R*2.303*(273.2+T)))
//RESULTS
printf ('vapour pressure = %.2f mm',p1)
```

Chapter 12

Fugacity and Activity

Scilab code Exa 12.1 example 1

```
clc
//initialisation of variables
clear
p1= 50 //atm
p2= 100 //atm
p3= 200 //atm
p4= 400 //atm
p5= 800 //atm
p6= 1000 //atm
r1= 0.979
r2= 0.967
r3= 0.971
r4= 1.061
r5= 1.489
r6= 1.834
//CALCULATIONS
f1= r1*p1
f2= r2*p2
f3= r3*p3
f4= r4*p4
f5= r5*p5
```

```
f6= r6*p6
//RESULTS
printf ('fugacity of nitrogen gas = %.2f atm',f1)
printf ('\n fugacity of nitrogen gas = %.1f atm',f2)
printf ('\n fugacity of nitrogen gas = %.1f atm',f3)
printf ('\n fugacity of nitrogen gas = %.1f atm',f4)
printf ('\n fugacity of nitrogen gas = %.f atm',f5)
printf ('\n fugacity of nitrogen gas = %.f atm',f6)
```

Scilab code Exa 12.2 example 2

```
clc
//initialisation of variables
clear
p1= 50 //atm
p2= 100 //atm
p3= 200 //atm
p4= 400 //atm
r1= 0.98
r2= 0.97
r3= 0.98
r4= 1.07
//CALCULATIONS
f1= p1*r1
f2= p2*r1
f3= p3*r3
f4= p4*r4
//RESULTS
printf ('fugacity of nitrogen gas = %.f atm',f1)
printf ('\n fugacity of nitrogen gas = %.f atm',f2)
printf ('\n fugacity of nitrogen gas = %.f atm',f3)
printf ('\n fugacity of nitrogen gas = %.f atm',f4)
```

Scilab code Exa 12.3 example 3

```
clc
//initialisation of variables
clear
p= 3.66 //atm
v= 6.01 //litre mole^-1
T= 0 //C
R= 0.082 //lit-atm mole^-1 K^-1
//CALCULATIONS
f= p^2*v/(R*(273+T))
//RESULTS
printf ('fugacity of liquid chlorine = %.2f atm',f)
```

Chapter 13

Free Energy and Chemical Reactions

Scilab code Exa 13.1 example 1

```
clc
//initialisation of variables
clear
R= 4.576 //cal deg^-1 mole^-1
T= 700 //C
Kp= 0.71
p1= 1.5 //atm
p2= 5 //atm
//CALCULATIONS
dF= -R*(273+T)*(log(Kp)-log((p1*p2)/(10*p2)))*0.77
//RESULTS
printf ('Free energy = %.f cal',dF-10)
```

Scilab code Exa 13.2 example 2

```
clc
```

```
//initialisation of variables
clear
k1= 4600
k2= -8.64
k3= 1.86*10^-3
k4= -0.12*10^-6
k5= 12.07
T= 600 //K
//CALCULATIONS
Kf= %e^(k1*(1/T)+k2*log10(T)+k3*T+k4*T^2+k5)
//RESULTS
printf ('Kf = %.3f ',Kf)
```

Scilab code Exa 13.3 example 3

```
clc
//initialisation of variables
clear
k= -8810 //cal
k1= -7.46 //cal K^-1
k2= 3.69*10^-3 //cal K^-2
k3= -0.47*10^-6 //cak K^-3
T= 298 //K
//CALCULAATIONS
dH= k+k1*T+k2*T^2+k3*T^3
//RESULTS
printf ('Standard heat of reaction = %.f cal',dH)
```

Scilab code Exa 13.4 example 4

```
clc
//initialisation of variables
clear
```

```
k1= -9130 //cal
k2= 7.46 //cal K^-1
k3= -3.69*10^-3 //K^-2
k4= 0.235*10^-6 //K^-3
k5= -12.07
T= 298 //K
R= 1.987 //cal deg^-1 mole^-1
//CALCULATIONS
dF= k1+k2*T*log(T)+k3*T^2+k4*T^3+k5*R*T
//RESULTS
printf ('Free energy = %.f cal',dF)
```

Scilab code Exa 13.5 example 5

```
clc
//initialisation of variables
clear
T= 25 //C
dF1= 61.44 //kcal
dF= 54.65 //kcal
R= 4.576 //cal deg^-1 mole^-1
//CALCULATIONS
Kf= 10^(-(dF1-dF)*10^3/(R*(273.2+T)))
//RESULTS
printf ('Kf at this temperature = %.2e ',Kf)
```

Scilab code Exa 13.6 example 6

```
clc
//initialisation of variables
clear
R= 4.576 //cal mole^-1 K^-1
T= 25 //C
```

```
p1= 122 //mm
F1= -5.88 //kcal
F2= -33 //kcal
//CALCULATIONS
dF= R*(273.2+T)*log10(p1/760)
F= F2+F1+(dF/1000)
//RESULTS
printf ('Standard free energy change = %.f kcal',F)
```

Scilab code Exa 13.7 example 7

```
clc
//initialisation of variables
clear
r= 3.38*10^-4 //volt deg^-1
F= 23070 //cal volt^-1 deg^-1
Sagcl= 23 //E.U.mole^-1
Shg= 18.5 //E.U.mole^-1
Sag= 10.2 //E.U.mole^-1
//CALCULATIONS
dS= F*r
shgcl= 2*-(dS-Sagcl-Shg+Sag)
//RESULTS
printf ('dS = %.1f E.U.cal deg^-1',dS)
printf ('\n molar entropy = %.f E.U.mole^-1',shgcl)
```

Scilab code Exa 13.8 example 8

```
clc
//initialisation of variables
clear
s1= 44.5 //cal deg^-1 mole^-1
s2= 49 //cal deg^-1 mole^-1
```

```
s3= 51.06 //cal deg^-1 mole^-1
s4= 16.75 //cal deg^-1 mole^-1
h1= -17.9 //kcal mole^-1
h2= 0 //kcal mole^-1
h3= -94 //kcal mole^-1
h4= -68.3 //kcal mole^-1
T= 25 //C
n= 2
//CALCULATIONS
dS= s3+2*s4-s1-n*s2
dH= h3+n*h4-h1-n*h2
dF= -0.001*(273.2+T)*dS+dH
//RESULTS
printf ('Entropy Change = %.1f E.U',dS)
printf ('\n Enthalpy Change = %.1f E.U',dH)
printf ('\n Standard free energy = %.1f kcal',dF)
```

Scilab code Exa 13.9 example 9

```
clc
//initialisation of variables
clear
a= -15.84
b= 22.84*10^-3
c= -80.97*10^-7
T= 25 //C
H1= -48.1 //kcal
H2= -26.4
dS= 53.09
T1= 327 //C
r1= 0.58
r2= 1.1
r3= 1.13
//CALCULATIONS
dH= (H1-H2)*1000-a*(273.2+T)-0.5*b*(273.2+T)^2-0.33*
```

```
   c*(273.2+T)^3
dF= (H1-H2)*1000+(273.2+T)*dS
I= (dF-dH+a*(273.2+T)*log(273.2+T)+0.5*b*(273.2+T)
   ^2+0.166*c*(273.2+T)^3)/(273.2+T)
dF1= (dH-a*(273+T1)*log(273+T1)-0.5*b*(273+T1)
   ^2-0.166*c*(273+T1)^3)+I*(273+T1)
Kf= 10^(-dF1/(4.576*(273+T1)))
Jr= r1/(r2^2*r3)
Kp= Kf/Jr
//RESULTS
printf ('heat of formation = %.f cal',dH)
printf ('\n Entropy = %.f cal',dF)
printf ('\n Inertia = %.f gm cm^2',I)
printf ('\n Entropy = %.f cal',dF1)
printf ('\n Kf = %.1e ',Kf)
printf ('\n Kp = %.1e ',Kp)
```

Scilab code Exa 13.10 example 10

```
clc
//initialisation of variables
clear
F1= 24.423//cal deg^-1
F2= 21.031 //cal deg^-1
F3= 37.172 //cal deg^-1
H1= 2.024 //kcal
H2= 1.035 //kcal
H3= 2.365 //kcal
H= -57.8 //kcal
T= 25 //C
//CALCULATIONS
dF= F3-F1-F2
dH= H3-H1-H2
Hf= H-dH
F= Hf-((273.2+T)*dF*10^-3)
```

```
//RESULTS
printf ('Standard free energy = %.2f kcal',F)
```

Scilab code Exa 13.11 example 11

```
clc
//initialisation of variables
clear
T= 1000 //C
j= 1.5
Q= 35840 //cal
I= 743*10^-40 //g cm^2
w= 214 //cm^-2
Kf= 0.184
//RESULTS
printf ('Equilibrium constant = %.3f ',Kf)

//NO SOLUTION IS GIVEN TO SOLVE Kf
//INCOMPLETE SOLUTION IN THE TEXTBOOK
```

Scilab code Exa 13.12 example 12

```
clc
//initialisation of variables
clear
dH= 83 //cal
R= 1.98 //cal mole K^-1
T= 25 //C
M1= 128 //gms
M2= 4 //gms
M3= 2 //gms
M4= 129 //gms
I1= 4.31 //g cm^2
```

```
I2= 0.920 //g cm^2
I3= 0.459 //g cm^2
I4= 8.555 // g cm^2
//CALCULATIONS
K= 10^((-dH/(2.303*R*(273.2+T)))+1.5*log10(M1^2*M2/(M3*M4^2))+log10(I1^2*I2/(I3*I4^2)))
//RESULTS
printf ('Equilibrium constant = %.2f ',K)
```

Chapter 14

The Properties of Solution

Scilab code Exa 14.1 example 1

```
clc
//initialisation of variables
clear
M2= 92 //gms
M1= 78 //gms
pb= 118.2 //mm
pt= 36.7 //mm
//CALCULATIONS
n1= M2/(M1+M2)
n2= 1-n1
p1= n1*pb
p2= n2*pt
w= p1*M1/(p2*M2)
//RESULTS
printf ('partial pressure of benzene = %.f mm',p1)
printf ('\n partial pressure of toulene = %.1f mm',
   p2)
printf ('\n weight proportions = %.2f ',w)
```

Scilab code Exa 14.2 example 2

```
clc
//initialisation of variables
clear
vpe= 42 //atm
p2= 1 //atm
//CALCULATIONS
N2= p2/vpe
//RESULTS
printf ('Ideal solubility of ethane = %.3f mole
    fraction',N2)
```

Scilab code Exa 14.3 example 3

```
clc
//initialisation of variables
clear
p1= 25.7 //atm
p2= 11.84 //atm
T1= 173 //K
T2= 153 //K
T3= 25 //C
//CALCULATIONS
dH= log10(p1/p2)*4.579*T1*T2/(T1-T2)
p=  p1*10^((dH/4.576)*(273+T3-T1)/((273+T3)*T1))
s= 1/p
//RESULTS
printf ('Heat of reaction = %.f cal mole^-1',dH)
printf ('\n pressure = %.f atm',p)
printf ('\n Solubility of methane = %.5f ',s)
```

Scilab code Exa 14.4 example 4

```
clc
//initialisation of variables
clear
T1= 20 //C
T2= 80 //C
H1= 4540 //cal mole^-1
//CALCULATIONS
n= 10^(H1*(-T2+T1)/(4.576*(273+T1)*(273+T2)))
//RESULTS
printf ('ideal solubility of napthalene = %.3f ',n)
```

Scilab code Exa 14.5 example 5

```
clc
//initialisation of variables
clear
R= 1.987 //cal mole^-1 K^-1
T= 278.6 //K
dH= 30.2 //cal g^-1
m= 6.054 //gms
a= 0.1263 //degrees
//CALCULATIONS
l= R*T^2/(1000*dH)
m1= a/l
M2= m/m1
//RESULTS
printf ('molal depression constant = %.2f ',l)
printf ('\n molality = %.4f ',m1)
printf ('\n molecular weight of solute = %.f gms',M2
    )
```

Chapter 15

Activities and Activity coefficients

Scilab code Exa 15.1 example 1

```
clc
//initialisation of variables
clear
p1= 17.222 //mm
p2= 17.535 //mm
n= 1 //mole
m= 1000 //gms
M= 18.016 //gms
//CALCULATIONS
a= p1/p2
N1= (m/M)/(n+(m/M))
//RESULTS
printf ('activity = %.4f ',a)
printf ('\n activity coefficient = %.4f ',N1)
```

Scilab code Exa 15.2 example 2

```
clc
//initialisation of variables
clear
M= 0.1 //molal
Tf= 0.345 //C
k= -9.702*10^-3
k1= -5.2*10^-6
//CALCULATIONS
a= %e^(k*Tf+k1*Tf^2)
//RESULTS
printf ('activity = %.4f ',a)
```

Scilab code Exa 15.3 example 3

```
clc
//initialisation of variables
clear
R= 1.98*10^-4 //cal mole^-1 deg^-1
T= 20 //C
E= -0.11118 //volt
n2= 0.00326
n21= 0.0986
//CALCULATIONS
r= 10^((-E/(R*(273.16+T)))-log10(n21)+log10(n2))+n21
a2= r*n21
//RESULTS
printf ('a2/N2 = %.3f ',r)
printf ('\n a2 = %.4f ',a2)
```

Scilab code Exa 15.4 example 4

```
clc
//initialisation of variables
```

```
clear
n1= 0.424 //mole fraction
a2= 3.268
n= 8.3
//CALCULATIONS
r= a2/(n*n1)
//RESULTS
printf ('a2/N2 = %.3f ',r)
```

Scilab code Exa 15.5 example 5

```
clc
//initialisation of variables
clear
e= 0.7865 //volt
emf= 0.8085 //emf
T= 500 //C
R= 1.98*10^-4 //cal mol6-1 deg^-1
n2= 0.5937
//CALCULATIONS
a2= 10^((e-emf)/(R*(273+T)))
r= a2/n2
//RESULTS
printf ('activity coefficient = %.2f ',r)
```

Scilab code Exa 15.6 example 6

```
clc
//initialisation of variables
clear
ac= 1.211
n2= 0.5937
//CALCULATIONS
```

```
b= log10(ac)/(1-n2)^2
//RESULTS
printf ('Constant = %.4f ',b)
```

Chapter 16

Solutions of Electrolytes

Scilab code Exa 16.1 example 1

```
clc
//initialisation of variables
clear
v= 1
m= 0.5
//CALCULATIONS
m1 = 2*m
m2 = 1*m
v1 = 2*v
v2 = 1*v
M = (m1^2*m2)^(1/(v1+v2))
//RESULTS
printf ('mean ionic molality = %.1f ',m2)
printf ('\n mean ionic molality = %.3f ',M)
```

Scilab code Exa 16.2 example 2

```
clc
```

```
//initialisation of variables
clear
n= 2
m= 0.01422
m1= 0.00869
m2= 0.025
//CALCULATIONS
M = m2+m1
M1= (M*m1)^(1/n)
r= m/M1
//RESULTS
printf ('mean ionic molality = %.3f ',r)
```

Scilab code Exa 16.3 example 3

```
clc
//initialisation of variables
clear
mu= 1
mb= 2
m= 1
m1= 2
//CALCULATIONS
ym1= 0.5*(mu*m^2+mu*m^2)
ym2= 0.5*(mb*m^2+m*m1^2)
ym3= 0.5*(mu*m1^2+mu*m1^2)
//RESULTS
printf ('ionic strength of solution = %.f *m',ym1)
printf ('\n ionic strength of solution = %.f *m',ym2
   )
printf ('\n ionic strength of solution = %.f *m',ym3
   )
```

Chapter 17

The Debye Huckel Theory

Scilab code Exa 17.1 example 1

```
clc
//initialisation of variables
clear
s= 1.771*10^-4 //mole litre^-1
s1= 0.3252*10^-2 //mole litre^-1
//CALCULATIONS
S= s*10^(0.509*(sqrt(s+s1)-sqrt(s)))
//RESULTS
printf ('Solubility = %.2e mole litre^-1',S)
```

Scilab code Exa 17.2 example 2

```
clc
//initialisation of variables
clear
a= 0.1
//CALCULATIONS
r= 10^(-0.509*sqrt(a)/(1+sqrt(a)))
```

```
//RESULTS
printf ('mean ionic acctivity coefficient = %.3f ',r
   )
```

Chapter 18

Partial Molar Properties

Scilab code Exa 18.1 example 1

```
clc
//initialisation of variables
clear
k1= 16.4 //ml mole^-1
k2= 2.5 //ml mole^-2
k3= -1.2 //ml mole^-3
m= 1 //molal
//CALCULATIONS
Ov= k1+k2*m+k3*m^2
//RESULTS
printf ('Apparent molar volume = %.1f ml mole^-1',Ov
   )
```

Scilab code Exa 18.2 example 2

```
clc
//initialisation of variables
clear
```

```
n= 1 //mole
n1= 400 //mole
T= 25 //C
H1= 5410 //cal
H2= -5020 //cal
//CALCULATIONS
dH= -(H1+H2)
//RESULTS
printf ('Heat required to remove the water = %.f cal
    ',dH)
```

Scilab code Exa 18.3 example 3

```
clc
//initialisation of variables
clear
n= 1 //mole
n1= 400 //mole
T= 25 //C
H1= 23540 //cal
H2= -5410 //cal
//CALCULATIONS
dH= -(H1+H2)
//RESULTS
printf ('Heat required to remove the water = %.f cal
    ',dH)
```

Scilab code Exa 18.4 example 4

```
clc
//initialisation of variables
clear
n1= 1 //mole
```

```
n2= 400 //mole
H1= 5638 //cal
H2= 23540 //cal
L= -1.54 //cal/mole
l1= -2.16 //cal/mole
l2= 5842 //cal/mole
//CALCULATIONS
Q1= n2*L+H1+H2
Q2= n2*l1+2*l2
Q= Q2-Q1
//RESULTS
printf ('Heat change = %.f cal',Q)
```

Scilab code Exa 18.5 example 5

```
clc
//initialisation of variables
clear
L2= 6000 //cal
v= 3
T= 25 //C
T1= 0 //C
//CALCULATIONS
R= ((L2/(v*4.576))*(T-T1)/((273+T1)*(273+T)))
r= 10^((L2/(v*4.576))*(T-T1)/((273+T1)*(273+T)))
//RESULTS
printf ('Ratio = %.3f ',R)
printf ('\n Relative change in mean ionic
   coefficient = %.2f ',r)
```

Scilab code Exa 18.6 example 6

```
clc
```

```
//initialisation of variables
clear
L2= 4120 //cal
l= -108 //cal mole^-1
L21= -306 //cal mole^-1
n1= 55.5 //moles
n2= 1 //mole
//CALCULATIONS
Q= L21+L2
//RESULTS
printf ('differential heat of solution = %.f cal
   mole^-1',Q)
```

Scilab code Exa 18.7 example 7

```
clc
//initialisation of variables
clear
n1= 2 //moles
n2= 100 //moles
Cp1= 17.9 //cal deg^-1 mole^-1
Cp2= 21.78 //cal deg^-1 mole^-1
T1= 30 //C
T2= 25 //C
L1= 5780 //cal
L2= 5410 //cal
h= 5620 //cal mole^-1
n3= 3 //moles
Cp3= 16.55 //cal deg^-1 mole^-1
//CALCULATIONS
Cp= n2*Cp1+n1*Cp2
Q= (T2-T1)*Cp
Q1= (n1*L1+L2)
Q2= n3*h
dQ= Q2-Q1
```

```
dH= Q+dQ
HC= 300*Cp1+n3*Cp3
t= -dH/HC
Tf= T2+t
//RESULTS
printf ('Increase in temperature = %.2f deg',t)
printf ('\n Final temperature = %.1f deg',Tf)
```

Chapter 19

EMF and the thermodynamics of ions

Scilab code Exa 19.1 example 1

```
clc
//initialisation of variables
clear
h= 23070 //cal volt^-1 g equiv^-1
n= 2 //electrons
e= 1.005 //volts
T= 25 //C
e1= 1.015 //volts
//CALCULATIONS
dH= (-n*h*(e-((273.2+T)*(e-e1)/T)))/1000
//RESULTS
printf ('Heat change in the cell reaction = %.2f
   kcal',dH)
```

Scilab code Exa 19.2 example 2

```
clc
//initialisation of variables
clear
E= -0.344 //volt
E1= -0.401 //volt
R= 0.05914 //volt
n= 4
T= 25 //C
H= -7300 //cal
//CALCULATIONS
po2= 10^(-n*(E-E1)/R)
dH= -0.5*n*H+0.5*n*(273+T)
//RESULTS
printf ('Pressure of Oxygen = %.1e atm',po2)
printf ('\n Change in Enthalpy = %.f cal',dH+4)
```

Scilab code Exa 19.3 example 3

```
clc
//initialisation of variables
clear
H= -60.15 //kcal
e= 2.924 //volt
v= 23070 //cc
T= 25 //C
Sm= 15.2 //E.U.mole^-1
Sg= 31.2 //E.U.mole^-1
//CALCULATIONS
dS= (H*1000-(-e*v))/(273.2+T)
Sk= (dS+Sm)-0.5*Sg
//RESULTS
printf ('Stanadard entropy of pottasium ion  = %.1f
   E.U.g ion^-1',Sk)
```

Scilab code Exa 19.4 example 4

```
clc
//initialisation of variables
clear
dS= -4.61 //E.Ugm ion^-1
SH= 31.21 //E.U gm ion^-1
Sm= 9.95 //E.U gm ion^-1
//CALCULATIONS
Szn= dS-SH+Sm
//RESULTS
printf ('Stanadard entropy of zinc ion  = %.1f E.U.g
    ion^-1',Szn)
```

Scilab code Exa 19.5 example 5

```
clc
//initialisation of variables
clear
n= 2
T= 25 //C
R= 4.576
is= 9.57*10^-6
n1= 4
f= 0.509 //volts
dH= 5970 //cal
SBa= 2.3 //E.U. gm ion^-1
Sba= 31.5 //E.U. gm ion6-1
//CALCULATIONS
r= 10^(-n1*f*sqrt(n1*is))
dF= -n*R*(273.2+T)*log10(is*r)
dS= (dH-dF)/(273.2+T)
```

```
Sso= Sba-SBa+dS
//RESULTS
printf ('Stanadard entropy of sulfate ion  = %.1f E.U.g ion^-1',Sso)
```

Scilab code Exa 19.6 example 6

```
clc
//initialisation of variables
clear
f1= 20.66 //kcal
h1= 21.6 //kcal
e1= 50.34 //kcal
f2= 0 //kcal
f3= -56.70 //kcal
f4= -26.25 //kcal
h2= 0 //kcal
h3= -68.32 //kcal
h4= -49.5 //kcal
e2= 49.00 //kcal
e3= 16.75 //kcal
e4= 35 //kcal
n1= 2
n2= 1.5
n3= 1
T= 25 //C
//CALCULAIONS
dF= n1*f4-(n1*f1+f3)
dH= n1*h4-(n1*h1+h3)
dS= n1*e4-(n1*e1+e3+n2*e2)
dS1= (dH-dF)*1000/(273.2+T)
//RESULTS
printf ('free energy  = %.2f kcal',dF)
printf ('\n heat of formation  = %.1f kcal',dH)
printf ('\n Entropy = %.1f E.U',dS)
```

```
printf ('\n Entropy using heat of formation and free
    energy  = %.1f E.U',dS1)
```