

Scilab Textbook Companion for
Thermodynamics for Chemists
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Book Description

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

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

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

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

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Chapter 1

Heat work and energy

Scilab code Exa 1.1 example 1

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

Scilab code Exa 1.2 example 1

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

```

3 clear
4 I= 0.565 //amp
5 R= 15.43 //ohms
6 t= 185 //secs
7 Tr= 0.544 //C
8 //CALCULATIONS
9 Q1= I^2*R*t
10 Q2= I^2*R*t/Tr
11 //RESULTS
12 printf ('Heat capacity = %.f int.joules deg^-1',Q2)

```

Scilab code Exa 1.3 example 3

```

1 clc
2 //initialisation of variables
3 clear
4 I= 0.565 //amp
5 R= 15.43 //ohms
6 t= 185 //secs
7 Tr= 0.544 //C
8 //CALCULATIONS
9 Q1= I^2*R*t
10 Q2= I^2*R*t/(Tr*4.183)
11 //RESULTS
12 printf ('Heat capacity = %.1f calories',Q2)

```

Scilab code Exa 1.4 example 4

```

1 clc
2 //initialisation of variables
3 clear
4 v= 1 //lit
5 p= 1 //atm

```

```

6 h= 76 //cm
7 d= 13.595 //kg/cm^3
8 g= 980.66 //dynes cm^-2
9 j= 4.18 //joules
10 //CALCULATIONS
11 W= v*p
12 W1= h*d*g
13 W2= W1*10^-4
14 W3= W2/j
15 //RESULTS
16 printf ('Work done in lit-atm = %.f lit-atm',W)
17 printf ('\n Work done in dynes = %.2e dynes cm^-2',
    W1)
18 printf ('\n Work done in ergs = %.2e ergs',W2)
19 printf ('\n Work done in calories = %.2f calories',
    W3)

```

Chapter 2

Properties of thermodynamic systems

Scilab code Exa 2.1 example 2

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

Scilab code Exa 2.2 example 2

```
1  clc
```

```

2 //initialisation of variables
3 clear
4 T= 0 //C
5 R= 0.0820 //lit-atm deg-1 mol-1
6 p= 400 //atm
7 //CALCULATIONS
8 V= R*(273+T)/p
9 //RESULTS
10 printf ('Volume of the ideal gas = %.4f lit mol-1',
    V)

```

Scilab code Exa 2.3 example 3

```

1 clc
2 //initialisation of variables
3 clear
4 p= 400 //atm
5 T= 273 //K
6 R= 0.0820 //lit-atm deg-1 mol-1
7 k= 1.27
8 //CALCULATIONS
9 V= k*R*T/p
10 //RESULTS
11 printf ('Volume of the ideal gas = %.4f lit mol-1',
    V)

```

Scilab code Exa 2.4 example 4

```

1 clc
2 //initialisation of variables
3 clear
4 V= 0.381 //lit
5 T= 313 //K

```

```

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

```

Scilab code Exa 2.5 example 5

```

1 clc
2 //initialisation of variables
3 clear
4 n1= 0.25 //mole
5 n2= 0.75 //mole
6 l= 0.0832 //lit
7 T= 50 //C
8 p1= 404 //atm
9 p2= 390 //atm
10 //CALCULATIONS
11 P= n1*p1+n2*p2
12 //RESULTS
13 printf ('Total Pressure = %.f atm ',P)

```

Scilab code Exa 2.6 example 6

```

1 clc
2 clear
3 //initialisation of variables
4 n1= 0.25 //mole
5 nh= 0.75 //mole

```

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

Chapter 3

The first law of thermodynamics

Scilab code Exa 3.1 example 1

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

Scilab code Exa 3.2 example 2

```

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

```

Chapter 4

Heat changes and heat capacities

Scilab code Exa 4.1 example 1

```
1  clc
2  //initialisation of variables
3  clear
4  T1= 400 //K
5  T2= 300 //K
6  k1= 6.095 //cal mole-1 K-1
7  k2= 3.253*10-3 //cal mole-1 K-2
8  k3= -1.017*10-6 //cal mole-1 K-3
9  //CALCULATIONS
10 dH= k1*(T1-T2)+0.5*k2*(T12-T22)+(1/3)*k3*(T13-T23)
11 //RESULTS
12 printf ('Heat required to raise the temperature = %.
    f cal-mole-1',dH)
```

Scilab code Exa 4.2 example 2

```

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

```

Scilab code Exa 4.3 example 3

```

1  clc
2  //initialisation of variables
3  clear
4  p1= 20 //atm
5  p2= 200 //atm
6  T1= 25 //C
7  n= 2/7
8  //CALCULATIONS
9  T2= (p1/p2)^n*(273+T1)-273
10 //RESULTS
11 printf ('Final temperature = %.f C',T2)

```

Scilab code Exa 4.4 example 4

```

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

```

```

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

```

Scilab code Exa 4.5 example 5

```

1 clc
2 //initialisation of variables
3 clear
4 Ti= 25 //C
5 p= 200 //atm
6 p= 1 //atm
7 dT= 31 //C
8 //CALCULATIONS
9 Tf= Ti-dT
10 //RESULTS
11 printf ('Final temperature = %.f degrees ',Tf)

```

Scilab code Exa 4.6 example 6

```

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

```

```

10 p= 10^-3
11 //CALCULATIONS
12 Cp= k1+k2*T+k3*T^2
13 dCp= k2+2*k3*T
14 dCp1= k4*p+k5*p
15 //RESULTS
16 printf ('Cp = %.2f cal deg^-1 mole^-1',Cp)
17 printf ('\n Specific heat at temperature = %.2e cal
    deg^-2 mole^-1',dCp)
18 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

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

Scilab code Exa 5.2 example 2

```
1  clc
2  //initialisation of variables
3  clear
4  H1= -337.3 //kcal
```

```

5 H2= -68.3 //kcal
6 H3= -372.8 //kcal
7 //CALCULATIONS
8 Ht= H1+H2-H3
9 //RESULTS
10 printf ('Heat change of reaction = %.1f kcal',Ht)

```

Scilab code Exa 5.3 example 3

```

1 clc
2 //initialisation of variables
3 clear
4 dH= -1228.2 //kcal
5 n1= 10
6 n2= 4
7 dH1= -94.05 //kcal
8 dH2= -68.32 //kcal
9 //CALCULATIONS
10 x= n1*dH1+n2*dH2-dH
11 //RESULTS
12 printf ('Heat of formation = %.1f kcal',x)

```

Scilab code Exa 5.4 example 4

```

1 clc
2 //initialisation of variables
3 clear
4 H1= -29.6 //kcal
5 H2= -530.6 //kcal
6 H3= -94 //kcal
7 H4= -68.3 //kcal
8 //CALCULATIONS
9 dH1= -(H1+H2-3*H3-4*H4)

```



```

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

```

Scilab code Exa 5.5 example 5

```

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

```

Scilab code Exa 5.6 example 6

```

1  clc
2  //initialisation of variables
3  clear
4  a= -2.776
5  b= 0.947*10^-3
6  c= 0.295*10^-6
7  T1= 373 //K

```

```

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

```

Scilab code Exa 5.7 example 7

```

1 clc
2 //initialisation of variables
3 clear
4 a1= 6.189
5 a2= 3.225
6 a3= 10.421
7 b1= 7.787*10-3
8 b2= 0.707*10-3
9 b3= -0.3*10-3
10 c1= -0.728*10-6
11 c2= -0.04014*10-6
12 c3= 0.7212*10-6
13 dH= -9.13 //kcal
14 //CALCULATIONS
15 a= -(a2+a3-a1)*10-3
16 b= -0.5*(b2+b3-b1)*10-3
17 c= -0.33*(c2+c3-c1)*10-3
18 //RESULTS
19 printf ('a = %.2e kcal mole-1',a)
20 printf ('\n b = %.2e kcal mole-1',b)
21 printf ('\n c = %.2e kcal mole-1',c)
22 printf ('\n dH = %.2f kcal mole-1',dH)

```

Scilab code Exa 5.8 example 8

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

Scilab code Exa 5.9 example 9

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

Scilab code Exa 5.10 example 10

```
1  clc
2  //initialisation of variables
3  clear
4  c1= 9.3 //cal deg-1
5  c2= 6.3 //cal deg-1
6  n= 2
7  dH= -57500 //cal
8  V= 3 //cc
9  v1= 3.5 //cc
10 T1= 25 //C
11 p1= 1 //atm
12 //CALCULATIONS
13 T2= (-dH/(c1+n*c2))+298
14 p2= p1*V*T2/(v1*(273+T1))
15 //RESULTS
16 printf ('Temperature final = %.f K',T2)
17 printf ('\n pressure final = %.1f atm ',p2)
```

Scilab code Exa 5.11 example 11

```
1  clc
2  //initialisation of variables
3  clear
4  Hc= 234.4 //kcal
5  Hdc= 300 //kcal
6  Hch= 436.5 //kcal
7  Hco= 152 //kcal
8  Hsco= 70 //kcal
9  Hoh= 110.2 //kcal
```

```

10 Hoo= 885 //kcal
11 Hb= 38 //kcal
12 Hc= 28 //kcal
13 Ha= 206 //kcal
14 H1co= 2128 //kcal
15 H1oh= 661 //kcal
16 H1c= 231 //kcal
17 //CALCULATIONS
18 dH= Hc+Hdc+Hch+Hco+Hsco+Hoh+Hoo+Ha+Hb+Hc-H1co-H1oh-
    H1c
19 //RESULTS
20 printf ( 'Heat of combustion = %.f kcal ',dH)

```

Chapter 6

Calculation of energy and heat capacity

Scilab code Exa 6.1 example 1

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

Scilab code Exa 6.2 example 2

```
1  clc
```

```

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

```

Scilab code Exa 6.3 example 3

```

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

```

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

Scilab code Exa 6.4 example 4

```
1 clc
2 //initialisation of variables
3 clear
4 h= 1.439
5 T= 300 //K
6 w= 4405 //cm-1
7 w1= 565 //cm-1
8 //CALCULATIONS
9 Qv1= (1-%e(-h*w/T))-1
10 Qv2= (1-%e(-h*w1/T))-1
11 //RESULTS
12 printf ( 'Vibrational Partition = %.3f ',Qv1)
13 printf ( '\n Vibrational Partition = %.3f ',Qv2)
```

Scilab code Exa 6.5 example 5

```
1 clc
2 //initialisation of variables
3 clear
4 h= 1.439
5 T= 300 //K
6 w= 565 //cm-1
7 R= 1.98 //cal /mol K
8 n= 0.56
9 //CALCULATIONS
10 Qr= h*w/T
11 Cv= n*R
12 //RESULTS
13 printf ( 'Vibrational Partition = %.2f ',Qr)
```



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

Scilab code Exa 6.6 example 6

```
1 clc
2 //initialisation of variables
3 clear
4 R= 1.986 //cal deg-1 mole-1
5 cv1= 0.392 //cal deg-1 mole-1
6 cv2= 0.004 //cal deg-1 mole-1
7 cv3= 0.003 //cal deg-1 mole-1
8 cv4= 1.265 //cal deg-1 mole-1
9 cv5= 0.247 //cal deg-1 mole-1
10 cv6= 0.225 //cal deg-1 mole-1
11 //CALCULATIONS
12 Cv = 3*R+cv1+cv2+cv3
13 Cv1= 3*R+cv4+cv5+cv6
14 //RESULTS
15 printf ( 'Total heat capacity = %.2f cal deg-1 mole
    ^-1', Cv)
16 printf ( '\n Total heat capacity = %.2f cal deg-1
    mole-1', Cv1)
```

Scilab code Exa 6.7 example 7

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

Scilab code Exa 6.8 example 8

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

Scilab code Exa 6.9 example 9

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

Chapter 7

The second law of thermodynamics

Scilab code Exa 7.1 example 1

```
1  clc
2  //initialisation of variables
3  clear
4  T1= 308 //K
5  T2= 373 //K
6  T3= 538 //K
7  //CALCULATIONS
8  e1= (T2-T1)/T2
9  e2= (T3-T1)/T3
10 //RESULTS
11 printf ('Efficiency = %.3f ',e1)
12 printf ('\n Efficiency = %.3f ',e2)
```

Scilab code Exa 7.2 example 2

```
1  clc
```

```

2 //initialisation of variables
3 clear
4 T= 25 //C
5 T1= 0 //C
6 h= 79.8 //cal g-1
7 j= 4.18*107 //ergs
8 //CALCULATIONS
9 Wc= (T-T1)*h/(273+T1)
10 W= (T-T1)*h*j/(273+T1)
11 //RESULTS
12 printf ('Work required = %.1f cal ',Wc)
13 printf ('\n Work required = %.2e ergs ',W)

```

Scilab code Exa 7.3 example 3

```

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

```

Chapter 8

Entropy relationships and applications

Scilab code Exa 8.1 example 1

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

Scilab code Exa 8.2 example 2

```

1  clc
2  //initialisation of variables
3  clear
4  T= 77.32 //K
5  p= 1 //atm
6  Tc = 126 //K
7  Pc= 33.5 //atm
8  Mo= 32 //gms
9  mo= 27 //gms
10 R= 1.98 //cal/mol K
11 //CALCULATIONS
12 dS= (mo)*R*Tc^3/(Mo*Pc*T^3)
13 //RESULTS
14 printf ('Entropy increase = %.3f cal deg-1',dS)

```

Scilab code Exa 8.3 example 3

```

1  clc
2  //initialisation of variables
3  R= 1.987 //cal deg-1 mole-1
4  T= 25 //C
5  Pc= 49.7 //atm
6  m= 128 //gms
7  pc= 49.7 //atm
8  Tc= 154.3 //K
9  m1= 9 //gms
10 m2= 18
11 //CALCULATIONS
12 dH= (m1*R*Tc/(m*pc))*(1-m2*(Tc/(273.15+T))^2)*-1
13 //RESULTS
14 printf ('Enthalpy = %.2f cal mole-1',dH)

```

Scilab code Exa 8.4 example 4

```

1  clc
2  //initialisation of variables
3  clear
4  a= 1.39 //lit^2
5  p= 200 //atm
6  R= 0.082 //lit-atm /mol K
7  T= 298 //K
8  //CALCULATIONS
9  dC= (1+(2*a*p/(R*T)^2))
10 //RESULTS
11 printf ('Cp-Cv = %.2f *R lit-atm mole^-1 K^-1 ',dC)

```

Scilab code Exa 8.5 example 5

```

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

```

Scilab code Exa 8.6 example 6

```

1  clc
2  //initialisation of variables
3  clear

```

```

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

```

Scilab code Exa 8.7 example 7

```

1 clc
2 //initialisation of variables
3 clear
4 p= 100 //atm
5 T= 25 //C
6 a= 1.38
7 b= 3.92*10^-2 //lit atm
8 R= 0.082 //lit-atm mole^-1 K^-1
9 Tc= 126 //K
10 Pc= 33.5 //atm
11 M= 81 //gms
12 m= 32 //gms
13 //CALCULATIONS
14 dC= a*2*p/(R*(273+T)^2)
15 dC1= M*R*Tc^3*p/(m*Pc*(273+T)^3)
16 //RESULTS
17 printf ('Cp-Cp* = %.3f lit atm deg^-1 mole^-1',dC)
18 printf ('\n Cp-Cp* = %.3f lit atm deg^-1 mole^-1',
    dC1)

```

Scilab code Exa 8.8 example 8


```

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

```

Scilab code Exa 8.9 example 9

```

1  clc
2  //initialisation of variables
3  clear
4  Cp= 8.21*0.0413 //lit-atm
5  R= 0.0821 //lit-atm deg-1 mole-1
6  p= 100 //atm
7  T= 20 //C
8  a= 1.39
9  b= 3.92*10-2 //lit-atm2 mole
10 //CALCULATIONS
11 u= (1/Cp)*((2*a/(R*(273+T)))-b-(3*a*b*p/(R2*(273+T)
    ^2)))
12 //RESULTS
13 printf ('Joule-thomson coefficient = %.3f deg atm-1
    ',u)

```

Chapter 9

Entropy determination and Significance

Scilab code Exa 9.1 example 1

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

Scilab code Exa 9.2 example 2

```
1  clc
```

```

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

```

Scilab code Exa 9.3 example 3

```

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

```

Scilab code Exa 9.4 example 4

```

1 clc
2 //initialisation of variables

```

```
3 clear
4 Sco= 47.3 //cal deg-1
5 Sh2= 31.21 //cal deg-1
6 Sc= 1.36 //cal deg-1
7 Sho = 16.75 //cal deg-1
8 //CALCULATIONS
9 S= Sco+Sh2-Sc-Sho
10 //RESULTS
11 printf ('Standard entropy = %.2f cal deg-1 mole-1'
        ,S)
```

Chapter 11

Phase Equilibria

Scilab code Exa 11.1 example 1

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

Scilab code Exa 11.2 example 2

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

```

3 clear
4 T= 95.5 //C
5 p= 1 //atm
6 v= 0.0126 //cc g-1
7 a= 0.0242 //cal cc-1 atm-1
8 r= 0.035 //K atm-1
9 //CALCULATIONS
10 dH= (273.2+T)*v*a/r
11 //RESULTS
12 printf ('Heat of transition = %.1f cal g-1',dH)

```

Scilab code Exa 11.3 example 3

```

1 clc
2 //initialisation of variables
3 clear
4 T= 100 //C
5 j= 0.0242 //cal cc-1 atm6-1
6 k= 539 //cal g-1
7 p= 1664 //cc g-1
8 //CALCULATIONS
9 r= (273.2+T)*(p-1)*j/k
10 //RESULTS
11 printf ('Rise in temperature per unit of pressure= %
    .1f deg atm-1',r)

```

Scilab code Exa 11.4 example 4

```

1 clc
2 //initialisation of variables
3 clear
4 T1= 100 //C
5 T2= 90 //C

```

```

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

```

Scilab code Exa 11.5 example 5

```

1 clc
2 //initialisation of variables
3 clear
4 T= 239.05 //K
5 r= 0.0242 //cal cc6-1 atm-1
6 Vv= 269.1 //cc g-1
7 Vl= 0.7 //cc g-1
8 r1= 3.343 //cm of mercury deg6-1
9 p= 76 //cm
10 //CALCULATIONS
11 tbyp= r1/p
12 dH= T*(Vv-Vl)*tbyp*r
13 //RESULTS
14 printf ('heat of vapourisation of liquid chlorine =
    %.1f cal g-1',dH)

```

Scilab code Exa 11.6 example 6

```

1 clc
2 //initialisation of variables
3 clear
4 Ta= 441 //C

```

```

5 Tb= 882 //C
6 Tb1= 1218 //C
7 //CALCULATIONS
8 Ta1= (273+Tb1)*(Tb+273)/(273+Ta)
9 Tb= Ta1-273
10 //RESULTS
11 printf ('Normal boiling point of silver = %.f K',Ta1
    )
12 printf ('\n Normal boiling point of silver in
    degrees = %.f degrees ',Tb)

```

Scilab code Exa 11.7 example 7

```

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

```

Scilab code Exa 11.8 example 8

```

1 clc
2 //initialisation of variables
3 clear
4 p= 23.76 //mm
5 R= 0.082 //atm-lit deg^-1 mol^-1
6 T= 25 //C
7 vl= 18 //ml

```



```

8  p1= 1 //atm
9  //CALCULATIONS
10 dP= 0.001*v1*p*p1/(R*(273+T))
11 p2= p+dP
12 //RESULTS
13 printf ('vapour pressure = %.2f mm',p2)
14
15 //ANSWER GIVEN IN THE TEXTBOOK IS WRONG

```

Scilab code Exa 11.9 example 9

```

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

```

Chapter 12

Fugacity and Activity

Scilab code Exa 12.1 example 1

```
1  clc
2  //initialisation of variables
3  clear
4  p1= 50 //atm
5  p2= 100 //atm
6  p3= 200 //atm
7  p4= 400 //atm
8  p5= 800 //atm
9  p6= 1000 //atm
10 r1= 0.979
11 r2= 0.967
12 r3= 0.971
13 r4= 1.061
14 r5= 1.489
15 r6= 1.834
16 //CALCULATIONS
17 f1= r1*p1
18 f2= r2*p2
19 f3= r3*p3
20 f4= r4*p4
21 f5= r5*p5
```

```

22 f6= r6*p6
23 //RESULTS
24 printf ('fugacity of nitrogen gas = %.2f atm',f1)
25 printf ('\n fugacity of nitrogen gas = %.1f atm',f2)
26 printf ('\n fugacity of nitrogen gas = %.1f atm',f3)
27 printf ('\n fugacity of nitrogen gas = %.1f atm',f4)
28 printf ('\n fugacity of nitrogen gas = %.f atm',f5)
29 printf ('\n fugacity of nitrogen gas = %.f atm',f6)

```

Scilab code Exa 12.2 example 2

```

1  clc
2  //initialisation of variables
3  clear
4  p1= 50 //atm
5  p2= 100 //atm
6  p3= 200 //atm
7  p4= 400 //atm
8  r1= 0.98
9  r2= 0.97
10 r3= 0.98
11 r4= 1.07
12 //CALCULATIONS
13 f1= p1*r1
14 f2= p2*r1
15 f3= p3*r3
16 f4= p4*r4
17 //RESULTS
18 printf ('fugacity of nitrogen gas = %.f atm',f1)
19 printf ('\n fugacity of nitrogen gas = %.f atm',f2)
20 printf ('\n fugacity of nitrogen gas = %.f atm',f3)
21 printf ('\n fugacity of nitrogen gas = %.f atm',f4)

```

Scilab code Exa 12.3 example 3

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

Chapter 13

Free Energy and Chemical Reactions

Scilab code Exa 13.1 example 1

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

Scilab code Exa 13.2 example 2

```
1  clc
```

```

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

```

Scilab code Exa 13.3 example 3

```

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

```

Scilab code Exa 13.4 example 4

```

1 clc
2 //initialisation of variables
3 clear

```

```

4 k1= -9130 //cal
5 k2= 7.46 //cal K-1
6 k3= -3.69*10-3 //K-2
7 k4= 0.235*10-6 //K-3
8 k5= -12.07
9 T= 298 //K
10 R= 1.987 //cal deg-1 mole-1
11 //CALCULATIONS
12 dF= k1+k2*T*log(T)+k3*T2+k4*T3+k5*R*T
13 //RESULTS
14 printf ('Free energy = %.f cal ',dF)

```

Scilab code Exa 13.5 example 5

```

1 clc
2 //initialisation of variables
3 clear
4 T= 25 //C
5 dF1= 61.44 //kcal
6 dF= 54.65 //kcal
7 R= 4.576 //cal deg-1 mole-1
8 //CALCULATIONS
9 Kf= 10-(dF1-dF)*103/(R*(273.2+T))
10 //RESULTS
11 printf ('Kf at this temperature = %.2e ',Kf)

```

Scilab code Exa 13.6 example 6

```

1 clc
2 //initialisation of variables
3 clear
4 R= 4.576 //cal mole-1 K-1
5 T= 25 //C

```

```

6 p1= 122 //mm
7 F1= -5.88 //kcal
8 F2= -33 //kcal
9 //CALCULATIONS
10 dF= R*(273.2+T)*log10(p1/760)
11 F= F2+F1+(dF/1000)
12 //RESULTS
13 printf ('Standard free energy change = %.f kcal',F)

```

Scilab code Exa 13.7 example 7

```

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

```

Scilab code Exa 13.8 example 8

```

1 clc
2 //initialisation of variables
3 clear
4 s1= 44.5 //cal deg^-1 mole^-1
5 s2= 49 //cal deg^-1 mole^-1

```



```

6  s3= 51.06 //cal deg-1 mole-1
7  s4= 16.75 //cal deg-1 mole-1
8  h1= -17.9 //kcal mole-1
9  h2= 0 //kcal mole-1
10 h3= -94 //kcal mole-1
11 h4= -68.3 //kcal mole-1
12 T= 25 //C
13 n= 2
14 //CALCULATIONS
15 dS= s3+2*s4-s1-n*s2
16 dH= h3+n*h4-h1-n*h2
17 dF= -0.001*(273.2+T)*dS+dH
18 //RESULTS
19 printf ('Entropy Change = %.1f E.U',dS)
20 printf ('\n Enthalpy Change = %.1f E.U',dH)
21 printf ('\n Standard free energy = %.1f kcal ',dF)

```

Scilab code Exa 13.9 example 9

```

1  clc
2  //initialisation of variables
3  clear
4  a= -15.84
5  b= 22.84*10-3
6  c= -80.97*10-7
7  T= 25 //C
8  H1= -48.1 //kcal
9  H2= -26.4
10 dS= 53.09
11 T1= 327 //C
12 r1= 0.58
13 r2= 1.1
14 r3= 1.13
15 //CALCULATIONS
16 dH= (H1-H2)*1000-a*(273.2+T)-0.5*b*(273.2+T)2-0.33*

```

```

        c*(273.2+T)^3
17 dF= (H1-H2)*1000+(273.2+T)*dS
18 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)
19 dF1= (dH-a*(273+T1)*log(273+T1)-0.5*b*(273+T1)
        ^2-0.166*c*(273+T1)^3)+I*(273+T1)
20 Kf= 10^(-dF1/(4.576*(273+T1)))
21 Jr= r1/(r2^2*r3)
22 Kp= Kf/Jr
23 //RESULTS
24 printf ('heat of formation = %.f cal ',dH)
25 printf ('\n Entropy = %.f cal ',dF)
26 printf ('\n Inertia = %.f gm cm^2 ',I)
27 printf ('\n Entropy = %.f cal ',dF1)
28 printf ('\n Kf = %.1e ',Kf)
29 printf ('\n Kp = %.1e ',Kp)

```

Scilab code Exa 13.10 example 10

```

1 clc
2 //initialisation of variables
3 clear
4 F1= 24.423 //cal deg^-1
5 F2= 21.031 //cal deg^-1
6 F3= 37.172 //cal deg^-1
7 H1= 2.024 //kcal
8 H2= 1.035 //kcal
9 H3= 2.365 //kcal
10 H= -57.8 //kcal
11 T= 25 //C
12 //CALCULATIONS
13 dF= F3-F1-F2
14 dH= H3-H1-H2
15 Hf= H-dH
16 F= Hf-((273.2+T)*dF*10^-3)

```

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

Scilab code Exa 13.11 example 11

```
1 clc
2 //initialisation of variables
3 clear
4 T= 1000 //C
5 j= 1.5
6 Q= 35840 //cal
7 I= 743*10^-40 //g cm^2
8 w= 214 //cm^-2
9 Kf= 0.184
10 //RESULTS
11 printf ('Equilibrium constant = %.3f ',Kf)
12
13 //NO SOLUTION IS GIVEN TO SOLVE Kf
14 //INCOMPLETE SOLUTION IN THE TEXTBOOK
```

Scilab code Exa 13.12 example 12

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

```

12 I2= 0.920 //g cm^2
13 I3= 0.459 //g cm^2
14 I4= 8.555 // g cm^2
15 //CALCULATIONS
16 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)))
17 //RESULTS
18 printf ('Equilibrium constant = %.2f ',K)

```

Chapter 14

The Properties of Solution

Scilab code Exa 14.1 example 1

```
1  clc
2  //initialisation of variables
3  clear
4  M2= 92 //gms
5  M1= 78 //gms
6  pb= 118.2 //mm
7  pt= 36.7 //mm
8  //CALCULATIONS
9  n1= M2/(M1+M2)
10 n2= 1-n1
11 p1= n1*pb
12 p2= n2*pt
13 w= p1*M1/(p2*M2)
14 //RESULTS
15 printf ('partial pressure of benzene = %.f mm',p1)
16 printf ('\n partial pressure of toluene = %.1f mm',
    p2)
17 printf ('\n weight proportions = %.2f ',w)
```

Scilab code Exa 14.2 example 2

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

Scilab code Exa 14.3 example 3

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

Scilab code Exa 14.4 example 4

```

1  clc
2  //initialisation of variables
3  clear
4  T1= 20 //C
5  T2= 80 //C
6  H1= 4540 //cal mole-1
7  //CALCULATIONS
8  n= 10^(H1*(-T2+T1)/(4.576*(273+T1)*(273+T2)))
9  //RESULTS
10 printf ('ideal solubility of naphthalene = %.3f ',n)

```

Scilab code Exa 14.5 example 5

```

1  clc
2  //initialisation of variables
3  clear
4  R= 1.987 //cal mole-1 K-1
5  T= 278.6 //K
6  dH= 30.2 //cal g-1
7  m= 6.054 //gms
8  a= 0.1263 //degrees
9  //CALCULATIONS
10 l= R*T2/(1000*dH)
11 m1= a/l
12 M2= m/m1
13 //RESULTS
14 printf ('molal depression constant = %.2f ',l)
15 printf ('\n molality = %.4f ',m1)
16 printf ('\n molecular weight of solute = %.f gms',M2
)

```

Chapter 15

Activities and Activity coefficients

Scilab code Exa 15.1 example 1

```
1  clc
2  //initialisation of variables
3  clear
4  p1= 17.222 //mm
5  p2= 17.535 //mm
6  n= 1 //mole
7  m= 1000 //gms
8  M= 18.016 //gms
9  //CALCULATIONS
10 a= p1/p2
11 N1= (m/M)/(n+(m/M))
12 //RESULTS
13 printf ('activity = %.4f ',a)
14 printf ('\n activity coefficient = %.4f ',N1)
```

Scilab code Exa 15.2 example 2


```

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

```

Scilab code Exa 15.3 example 3

```

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

```

Scilab code Exa 15.4 example 4

```

1  clc
2  //initialisation of variables

```

```

3 clear
4 n1= 0.424 //mole fraction
5 a2= 3.268
6 n= 8.3
7 //CALCULATIONS
8 r= a2/(n*n1)
9 //RESULTS
10 printf ( 'a2/N2 = %.3f ',r)

```

Scilab code Exa 15.5 example 5

```

1 clc
2 //initialisation of variables
3 clear
4 e= 0.7865 //volt
5 emf= 0.8085 //emf
6 T= 500 //C
7 R= 1.98*10^-4 //cal mol-1 deg-1
8 n2= 0.5937
9 //CALCULATIONS
10 a2= 10^((e-emf)/(R*(273+T)))
11 r= a2/n2
12 //RESULTS
13 printf ( 'activity coefficient = %.2f ',r)

```

Scilab code Exa 15.6 example 6

```

1 clc
2 //initialisation of variables
3 clear
4 ac= 1.211
5 n2= 0.5937
6 //CALCULATIONS

```

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

Chapter 16

Solutions of Electrolytes

Scilab code Exa 16.1 example 1

```
1  clc
2  //initialisation of variables
3  clear
4  v= 1
5  m= 0.5
6  //CALCULATIONS
7  m1 = 2*m
8  m2 = 1*m
9  v1 = 2*v
10 v2 = 1*v
11 M = (m1^2*m2)^(1/(v1+v2))
12 //RESULTS
13 printf ('mean ionic molality = %.1f ',m2)
14 printf ('\n mean ionic molality = %.3f ',M)
```

Scilab code Exa 16.2 example 2

```
1  clc
```

```

2 //initialisation of variables
3 clear
4 n= 2
5 m= 0.01422
6 m1= 0.00869
7 m2= 0.025
8 //CALCULATIONS
9 M = m2+m1
10 M1= (M*m1)^(1/n)
11 r= m/M1
12 //RESULTS
13 printf ('mean ionic molality = %.3f ',r)

```

Scilab code Exa 16.3 example 3

```

1 clc
2 //initialisation of variables
3 clear
4 mu= 1
5 mb= 2
6 m= 1
7 m1= 2
8 //CALCULATIONS
9 ym1= 0.5*(mu*m^2+mu*m^2)
10 ym2= 0.5*(mb*m^2+m*m1^2)
11 ym3= 0.5*(mu*m1^2+mu*m1^2)
12 //RESULTS
13 printf ('ionic strength of solution = %.f *m',ym1)
14 printf ('\n ionic strength of solution = %.f *m',ym2
)
15 printf ('\n ionic strength of solution = %.f *m',ym3
)

```

Chapter 17

The Debye Huckel Theory

Scilab code Exa 17.1 example 1

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

Scilab code Exa 17.2 example 2

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

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

Chapter 18

Partial Molar Properties

Scilab code Exa 18.1 example 1

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

Scilab code Exa 18.2 example 2

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



```

4  n= 1 //mole
5  n1= 400 //mole
6  T= 25 //C
7  H1= 5410 //cal
8  H2= -5020 //cal
9  //CALCULATIONS
10 dH= -(H1+H2)
11 //RESULTS
12 printf ('Heat required to remove the water = %.f cal
        ',dH)

```

Scilab code Exa 18.3 example 3

```

1  clc
2  //initialisation of variables
3  clear
4  n= 1 //mole
5  n1= 400 //mole
6  T= 25 //C
7  H1= 23540 //cal
8  H2= -5410 //cal
9  //CALCULATIONS
10 dH= -(H1+H2)
11 //RESULTS
12 printf ('Heat required to remove the water = %.f cal
        ',dH)

```

Scilab code Exa 18.4 example 4

```

1  clc
2  //initialisation of variables
3  clear
4  n1= 1 //mole

```

```

5 n2= 400 //mole
6 H1= 5638 //cal
7 H2= 23540 //cal
8 L= -1.54 //cal/mole
9 l1= -2.16 //cal/mole
10 l2= 5842 //cal/mole
11 //CALCULATIONS
12 Q1= n2*L+H1+H2
13 Q2= n2*l1+2*l2
14 Q= Q2-Q1
15 //RESULTS
16 printf ('Heat change = %.f cal',Q)

```

Scilab code Exa 18.5 example 5

```

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

```

Scilab code Exa 18.6 example 6

```

1 clc

```

```

2 //initialisation of variables
3 clear
4 L2= 4120 //cal
5 l= -108 //cal mole-1
6 L21= -306 //cal mole-1
7 n1= 55.5 //moles
8 n2= 1 //mole
9 //CALCULATIONS
10 Q= L21+L2
11 //RESULTS
12 printf ('differential heat of solution = %.f cal
    mole-1',Q)

```

Scilab code Exa 18.7 example 7

```

1 clc
2 //initialisation of variables
3 clear
4 n1= 2 //moles
5 n2= 100 //moles
6 Cp1= 17.9 //cal deg-1 mole-1
7 Cp2= 21.78 //cal deg-1 mole-1
8 T1= 30 //C
9 T2= 25 //C
10 L1= 5780 //cal
11 L2= 5410 //cal
12 h= 5620 //cal mole-1
13 n3= 3 //moles
14 Cp3= 16.55 //cal deg-1 mole-1
15 //CALCULATIONS
16 Cp= n2*Cp1+n1*Cp2
17 Q= (T2-T1)*Cp
18 Q1= (n1*L1+L2)
19 Q2= n3*h
20 dQ= Q2-Q1

```

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

Chapter 19

EMF and the thermodynamics of ions

Scilab code Exa 19.1 example 1

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

Scilab code Exa 19.2 example 2

```

1  clc
2  //initialisation of variables
3  clear
4  E= -0.344 //volt
5  E1= -0.401 //volt
6  R= 0.05914 //volt
7  n= 4
8  T= 25 //C
9  H= -7300 //cal
10 //CALCULATIONS
11 po2= 10^(-n*(E-E1)/R)
12 dH= -0.5*n*H+0.5*n*(273+T)
13 //RESULTS
14 printf ('Pressure of Oxygen = %.1e atm',po2)
15 printf ('\n Change in Enthalpy = %.f cal ',dH+4)

```

Scilab code Exa 19.3 example 3

```

1  clc
2  //initialisation of variables
3  clear
4  H= -60.15 //kcal
5  e= 2.924 //volt
6  v= 23070 //cc
7  T= 25 //C
8  Sm= 15.2 //E.U. mole-1
9  Sg= 31.2 //E.U. mole-1
10 //CALCULATIONS
11 dS= (H*1000-(-e*v))/(273.2+T)
12 Sk= (dS+Sm)-0.5*Sg
13 //RESULTS
14 printf ('Stanadard entropy of pottasium ion = %.1f
    E.U. g ion-1',Sk)

```

Scilab code Exa 19.4 example 4

```
1  clc
2  //initialisation of variables
3  clear
4  dS= -4.61 //E.Ugm ion-1
5  SH= 31.21 //E.U gm ion-1
6  Sm= 9.95 //E.U gm ion-1
7  //CALCULATIONS
8  Szn= dS-SH+Sm
9  //RESULTS
10 printf ('Stanadard entropy of zinc ion = %.1f E.U.g
    ion-1', Szn)
```

Scilab code Exa 19.5 example 5

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

```

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

```

Scilab code Exa 19.6 example 6

```

1  clc
2  //initialisation of variables
3  clear
4  f1= 20.66 //kcal
5  h1= 21.6 //kcal
6  e1= 50.34 //kcal
7  f2= 0 //kcal
8  f3= -56.70 //kcal
9  f4= -26.25 //kcal
10 h2= 0 //kcal
11 h3= -68.32 //kcal
12 h4= -49.5 //kcal
13 e2= 49.00 //kcal
14 e3= 16.75 //kcal
15 e4= 35 //kcal
16 n1= 2
17 n2= 1.5
18 n3= 1
19 T= 25 //C
20 //CALCULAIONS
21 dF= n1*f4-(n1*f1+f3)
22 dH= n1*h4-(n1*h1+h3)
23 dS= n1*e4-(n1*e1+e3+n2*e2)
24 dS1= (dH-dF)*1000/(273.2+T)
25 //RESULTS
26 printf ('free energy = %.2f kcal ',dF)
27 printf ('\n heat of formation = %.1f kcal ',dH)
28 printf ('\n Entropy = %.1f E.U',dS)

```



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