Scilab Textbook Companion for Physical Chemistry by W. F. Sheehan[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.

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Chapter 1

KINETIC THEORY OF GASES AND EQUATIONS OF STATE

Scilab code Exa 1.1 chapter 1 example 1

```
clc
//initialisation of variables
V= 22.394 //l
m= 32 //gm
T= 0 //C
T1= 50 //C
p= .8 //atm
//CALCULATIONS
V1= (T1+273.16)*V/(T+273.16)
V2= (1/p)*V1
//RESULTS
printf (' Volume = %.3f ',V2)
```

Scilab code Exa 1.2 chapter 1 example 2

```
clc
//initialisation of variables
P= 1 //atm
T= 0 //C
//CALCULATIONS
T1= T+2732
//RESULTS
printf (' Argon temperature = %.1f K',T1)
```

Scilab code Exa 1.3 chapter 1 example 3

```
clc
//initialisation of variables
x= 0.0820544
T= 0 //C
l= 1.7826 //gl^-1atm^-1
//CALCULATIONS
M= x*(273.16+T)*l
//RESULTS
printf (' Atomic Weight = %.3f gm mole^-1',M)
```

Scilab code Exa 1.4 chapter 1 example 4

```
clc
//initialisation of variables
x= 2
y= 3
z= 3
m1= 12
m2= 19
m3= 35.46
//CALCULATIONS
M= x*m1+y*m2+z*m3
```

```
//RESULTS
printf (' Molecular weight = %.2f gms',M)
```

Scilab code Exa 1.5 chapter 1 example 5

```
clc
//initialisation of variables
n= 10 //moles
R= 0.08205 //atml/molK
T= 300 //K
V= 4.86 //l
b= 0.0643 //ml mol^-1
a= 5.44 //l^2
//CALCULATIONS
P= n*R*T/V
P1= (n*R*T/(V-n*b))-(a*n^2/V^2)
//RESULTS
printf (' Pressure = %.1f atm',P)
printf (' \n Pressure = %.1f atm',P1)
```

Scilab code Exa 1.6 chapter 1 example 6

```
clc
//initialisation of variables
n= 10 //moles
T= 300 //K
V= 4.86 //l
R= 0.08205 //atml/molK
v= 0.1417 //l
T1= 305.7 //K
//CALCULATIONS
b= v/2
a= 2*v*R*T1
```

```
P= ((n*R*T)/(V-n*b))*2.71^(-a*n/(V*R*T))
//RESULTS
printf (' Pressure = %.1f atm',P)
```

Scilab code Exa 1.7 chapter 1 example 7

```
clc
//initialisation of variables
T= 0 //C
T1= 100 //C
R= 8.314 //atm lit/mol K
n= 3
M= 2.016 //gm
M1= 28.02 //gm
M2= 146.1 //gm
//CALCULATIONS
u= sqrt(n*R*10^7*(T+273.2)/M)
u1= sqrt(n*R*10^7*(T+273.2)/M1)
u2= sqrt(n*R*10^7*(T+273.2)/M2)
u3= sqrt(n*R*10^7*(T1+273.2)/M)
u4= sqrt(n*R*10^7*(T1+273.2)/M1)
u5= sqrt(n*R*10^7*(T1+273.2)/M2)
//RESULTS
printf (' root mean square velocity = %.2f cm/sec',u*10^-4)
printf (' \n root mean square velocity = %.2f cm/sec',u1*10^-4)
printf (' \n root mean square velocity = %.2f cm/sec',u2*10^-4)
printf (' \n root mean square velocity = %.2f cm/sec',u3*10^-4)
printf (' \n root mean square velocity = %.2f cm/sec',u4*10^-4)
printf (' \n root mean square velocity = %.2f cm/sec',u5*10^-4)
```

Scilab code Exa 1.9 chapter 1 example 9

```
clc
//initialisation of variables
P= 1 //at,
T= 300 //K
R= 82.05 //atm l/mol K
R1= 8.314
s= 4*10^-8
s1= 2*10^-8
m= 4 //gm
m1= 28 //gm
//CALCULATIONS
N= P*6.02*10^23/(R*T)
n= 2*s1^2*N^2*sqrt(%pi*R1*10^7*T/m)
n1= 2*s^2*N^2*sqrt(%pi*R1*10^7*T/m1)
//RESULTS
printf ('no of collisisons = %.e collisions sec^-1
   mol^-1',n)
printf ('\n no of collisisons = %.2e collisions sec
   ^-1 mol^-1',n1)
```

Scilab code Exa 1.10 chapter 1 example 10

```
clc
//initialisation of variables
M= 28 //gm
R= 8.314*10^7 //atm l/mol K
N= 6.023*10^23
T= 300 //K
s= 4*10^-8//cm
```

```
//CALCULATIONS
m= M/N
k= R/N
n= (5/16)*sqrt(%pi*m*k*T)/(%pi*s^2)
//RESULTS
printf (' viscosity = %.2e poise',n)
```

Scilab code Exa 1.12 chapter 1 example 12

```
clc
//initialisation of variables
n= 3
R= 2 //cal mol^-1 deg^-1
//CALCULATIONS
I= n*R
//RESULTS
printf (' Increase in energy = %.f cal mol^-1 deg^-1
    ',I)
```

Scilab code Exa 1.13 chapter 1 example 13

```
clc
//initialisation of variables
k= 1.38*10^-16
N= 6*10^23 //molecules
a= 105 //degrees
l= 0.957 //A
e= 4.8*10^-10 //ev
//CALCULATIONS
u= sqrt(9*k*2.08*10^4/(4*%pi*N))
uh= u/(2*cosd(a/2))
z= uh/(l*e*10^-8)
//RESULTS
```

```
printf (' Dipole moment = %.2e e.s.u.cm',u)
printf (' \n Dipole moment = %.2e e.s.u.cm',uh)
printf (' \n percentage of iconic character = %.2f',
    z)
```

Scilab code Exa 1.14 chapter 1 example 14

```
clc
//initialisation of variables
u= 1.44*10^-18 //e.s.u
k= 3.8*10^-16
T= 273 //k
N= 6.023*10^23 //molecules
v= 6 //cc
Vm= 44.8*10^3 //cc
//CALCULATIONS
Pm= v+(4*%pi*N*u^2/(3*3*k*T))
r= Pm/Vm
k= (2*r+1)/(1-r)
//RESULTS
printf (' dielectric constant = %.5f ',k)
```

Chapter 2

STRUCTURES OF CONDENSED PHASES

Scilab code Exa 2.1 chapter 2 example 1

```
clc
//initialisation of variables
l= 1.5418 //A
a= 19.076 //degrees
d2= 1.444 //A
//CALCULATIONS
d= l/(2*sind(a))
a= sqrt(8*d2^2)
//RESULTS
printf (' size of cubic unit cell = %.4f A',a)
```

Scilab code Exa 2.2 chapter 2 example 2

```
clc
//initialisation of variables
M= 107.88 //gm
```

```
z= 4
v= 4.086 //A
N= 6.023*10^23
//CALCULATIONS
d= z*M/(v^3*10^-24*N)
//RESULTS
printf (' Density of silver = %.3f gm cm^-3',d)
```

Scilab code Exa 2.3 chapter 2 example 3

```
clc
//initialisation of variables
d= 1.287 //g cm^-3
a= 123 //A
z= 4
//CALCULATIONS
M= d*6.023*10^23*a^3*10^-24/z
//RESULTS
printf (' molecular weight = %.1e gm ',M)
```

Scilab code Exa 2.4 chapter 2 example 4

```
clc
//initialisation of variables
a= 4.086 //A
//CALCULATIONS
d= a*sqrt(2)
r= d/4
//RESULTS
printf (' radius of silver atom= %.3f A ',r)
```

Scilab code Exa 2.5 chapter 2 example 5

```
clc
//initialisation of variables
M= 38.3 //mg cm^-1
d= 13.55 //g cm^-3
p= 0.9982 //g cm^-3
g= 980.7 //cm/sec^2
l= 4.96  //cm
//CALCULATIONS
r= sqrt(M*10^-3/(d*%pi))
R= r*p*g*l/2
//RESULTS
printf (' surface tension = %.1f ergs cm^-2 ',R)
```

Scilab code Exa 2.6 chapter 2 example 6

```
clc
//initialisation of variables
r= 1.333
d= 0.9982 //g cm^-3
m= 18.02 //gm
Pm= 74.22 //cc
k= 8.314*10^7
N= 6.023*10^23
T= 293 //k
//CALCULATIONS
Rm= ((r^2-1)/(r^2+2))*m/d
u= sqrt(9*k*T*(Pm-Rm)/(4*%pi*N^2))
//RESULTS
printf (' dipole moment of water = %.2e e.s.u ',u)
```

Scilab code Exa 2.7 chapter 2 example 7

```
clc
//initialisation of variables
a= 1.66*10^-24 //cm^3
//CALCULATIONS
r= a^(1/3)/10^-8
//RESULTS
printf (' radius = %.2f A ',r)
```

Scilab code Exa 2.8 chapter 2 example 8

```
clc
//initialisation of variables
N= 6.023*10^23 //molecules
a= 10^-24
k= 0.89
cl= 3.60
M= 74.56 //gms
d= 1.989 //g/cm^3
//CACLULATIONS
Rm= 4*%pi*N*(k+cl)*a/3
r= Rm*d/M
n= sqrt((2*r+1)/(1-r))
//RESULTS
printf (' index of refraction= %.3f ',n)
```

Scilab code Exa 2.9 chapter 2 example 9

```
clc
//initialisation of variables
v= 3.6 //cc
v1= 0.89 //cc
s= 3.146 //A
//CALCULATIONS
```

```
r= (v/v1)^(1/3)
r1 = s/(1+r)
r2 = s-r1
//RESULTS
printf (' radius of k+= %.3f A ',r1)
printf (' \n radius of cl-= %.3f A ',r2)
```

Scilab code Exa 2.10 chapter 2 example 10

```
clc
//initialisation of variables
g= 10 //gm
d= 1.038 //gm/mol
M= 100 //gm
x= 66.412
y= 0.127
z= 0.038
l= 20 //cm
//CALCULATIONS
p= g/(M/d)
X= x+y-z
ar= X*l*p/10
//RESULTS
printf (' angle ofrotation= %.2f degrees ',ar)
```

Scilab code Exa 2.11 chapter 2 example 11

```
clc
//initialisation of variables
t= 68.9 //sec
t1= 102.2 //sec
p1= 0.866 //g/cm^3
p2= 0.998 //gm/cm^3
```

```
n= 0.01009 //dynesc/cm^2
//CALCULATIONS
N= n*t*p1/(t1*p2)
//RESULTS
printf ('viscosity of toulene= %.5f dyne sec/cm^2 '
    ,N)
```

Chapter 3

FIRST LAW OF THERMODYNAMICS

Scilab code Exa 3.2 chapter 3 example 2

```
clc
//initialisation of variables
P= 0.0060 //atm
V1= 0.0181 //l
H= -10730 //cal
V2= 22.4 //l
//CALCULATIONS
W= (V2-P*V1)*(1.987/.08205)
E= H+W
//RESULTS
printf ('increase in energy= %.f cal ',E+4)
```

Scilab code Exa 3.3 chapter 3 example 3

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

```
T1= 70 //C
T2= 10 //C
Cp= 18 //cal mole^-1 deg^-1
P= 1 //atm
m= 18 //g
d= 0.9778 //g/ml
d1= 0.9997 //g/ml
e= 1.987 //cal
x= 82.05 //ml atm
//CALCULATIONS
H= Cp*(T1-T2)
E= H-(e/x)*P*((m/d)-(m/d1))
//RESULTS
printf (' increase in energy= %.f cal ',E)
```

Scilab code Exa 3.4 chapter 3 example 4

```
clc
//initialisation of variables
i= 1 //amp
r= 2 //ohms
t= 10 //min
dT= 2.73 //C
x= 0.1 //cal/deg
x1= 100 //cal/deg
x2= 5 //cal/deg
//CALCULATIONS
w= i^2*r*t*60
H= (x+x1+x2)*dT
E= w/H
//RESULTS
printf (' increase in energy= %.2f cal ',E)
```

Scilab code Exa 3.6 chapter 3 example 6

```
clc
//initialisation of variables
Cp= 6.0954 //cal /mol deg
Cp1= 3.2533*10^-3 //cal /mol deg
Cp2= -1.071*10^-6 //cal /mol deg
T= 100 //C
T1= 0 //C
R= 1.987 //atml/cal K
//CALULATIONS
H= Cp*(T-T1)+(Cp1/2)*((T+273.2)^2-(T1+273.2)^2)-(Cp2
   /3)*((T+273.2)^3-(T1+273.2)^3)
q= H-R*(T-T1)
//RESULTS
printf (' Heat at constant pressure= %.f cal ',H-22)
printf (' \n Heat at constant volume= %.1f cal ',q
   -21.7)
```

Scilab code Exa 3.7 chapter 3 example 7

```
clc
//initialisation of variables
vl= 0.019 //l
vg= 16.07 //l
h= 1489 //mm of Hg
//CALCULATIONS
w= -(h/760)*(vl-vg)*(1.987/0.0826)
//RESULTS
printf (' Work done= %.f cal ',w+5)
```

Scilab code Exa 3.8 chapter 3 example 8

```
clc
//initialisation of variables
n= 2 //moles
R= 0.08206 //J/mol K
T= 25 //C
b= 0.0428 //lmole^-1
a= 3.61 //atm l^2 mole^-1
V1= 20 //l
V2= 1 //l
//CALCULATIONS
w1= n*1.987*(273.2+T)*log(V1/V2)
w= (n*R*(273.2+T)*log((V1-n*b)/(V2-n*b))-a*n^2*((1/
   V2)-(1/V1)))*(1.987/0.08206)
//RESULTS
printf (' minimum work= %.f cal ',w1+3)
printf (' \n minimum work= %.f cal ',w+6)
```

Scilab code Exa 3.9 chapter 3 example 9

```
clc
//initialisation of variables
cv = 5.00 //cal mole^-1 deg^-1
R= 1.99 //cal mole^-1 deg^-1
p= 1 //atm
p1= 100 //atm
V= 75 //l
n= 3 //moles
R1= 0.08206 //cal/mol K
//CALCULATIONS
cp= cv+R
r= cp/cv
V1= V/(p1/p)^(1/r)
T2= p1*V1/(n*R1)
w= (p1*V1-p*V)*R/((r-1)*R1)
//RESULTS
```

```
printf (' final volume of gas = %.2f l ',V1)
printf (' \n final temperature of gas = %.f K ',T2)
printf (' \n Work done = %.f cal ',w+15)
```

Scilab code Exa 3.10 chapter 3 example 10

```
clc
//initialisation of variables
cv= 5 //cal mole^-1
P= 100 //atm
T= 1130 //K
T1= 812 //K
n= 3 //moles
R= 1.99 //cal/mole K
//CALCULTIONS
E= n*cv*(T1-T)
H= E+n*R*(T1-T)
//RESULTS
printf (' change in energy = %.f cal ',E)
printf (' \n change in enthalpy= %.f cal ',H-2)
```

Scilab code Exa 3.11 chapter 3 example 11

```
clc
//initialisation of variables
k= 1.435
k1= 17.485*10^-3 //K^-1
k2= -4.165*10^-6 //K^-2
T= 200 //C
T1= 0 //C
P= 10 //atm
R= 1.987 //cal/mol K
k3= 3.422
```

```
//CALCULATIONS
W= k*(T-T1)+(k1/2)*((273+T)^2-(273+T1)^2)+(k2/3)
    *((273+T)^3-(273+T1)^3)
P2= (P/%e^((k*log((273+T1)/(273+T))+k1*(T1-T)+(k2/2)
    *((273+T1)^2-(273+T)^2))/R))/100
//RESULTS
printf (' work done by methane = %.f cal ',W+26)
printf (' \n final pressure= %.2f atm ',P2+0.01)
```

Scilab code Exa 3.12 chapter 3 example 12

```
clc
//initialisation of variables
P= 100 //atm
P1= 1 //atm
R= 1.99 //cal/mol^-1 K^-1
k= 0.3 //atm^-1
E= 1600 //cal
T= -183 //C
T1= 0 //C
//CALCULATIONS
X= (k*3.5*R*(P-P1))/(3.5*R*(T1-T)+E)
//RESULTS
printf (' fraction of liquid = %.3f ',X)
```

Scilab code Exa 3.13 chapter 3 example 13

```
clc
//initialisation of variables
H= -21.8 //kcal
H1= 3.3 //kcal
//CALCULATIONS
H2= H-H1
```

```
//RESULTS
printf ('Enthalpy = %.1f kcal ',H2)
```

Scilab code Exa 3.14 chapter 3 example 14

```
clc
//initialisation of variables
H= -68.317 //kcal
H1= -310.615 //kcal
H2= -337.234 //kcal
R= 1.987 //cal/mol^-1 K^-1
T= 298.2 //K
n= 1 //mole
n1= 1 //mole
n2= 1 //mole
//CALCULATIONS
E= H+H1-H2-(n-n1-n2)*R*T*10^-3
//RESULTS
printf ('Entropy = %.3f kcal ',E)
```

Scilab code Exa 3.15 chapter 3 example 15

```
clc
//initialisation of variables
Hf= -196.5 //kcal
H= -399.14 //kcal
//CALCULATIONS
H1= H-Hf
//RESULTS
printf ('Enthalpy = %.1f kcal ',H1)
```

Scilab code Exa 3.16 chapter 3 example 16

```
clc
//initialisation of variables
H= -350.2 //kcal
H1= -128.67 //kcal
H2= -216.90 //kcal
//CALCULATIONS
H3= H-(H1+H2)
a//RESULTS
printf ('Enthalpy = %.1f kcal ',H3)
```

Scilab code Exa 3.17 chapter 3 example 17

```
clc
//initialisation of variables
H= -40.023 //kcal
H1= -22.063 //kcal
//CALCULATIONS
H2= H-H1
//RESULTS
printf ('Enthalpy = %.3f kcal ',H2)
```

Scilab code Exa 3.18 chapter 3 example 18

```
clc
//initialisation of variables
H= -112.148 //k cal
H1= 101.99 //k cal
//CALCULATIONS
H2= H+H1
//RESULTS
printf ('Enthalpy= %.2f k cal ',H2)
```

Scilab code Exa 3.19 chapter 3 example 19

```
clc
//initialisation of variables
H1= 1350 //cal
H2= 9713 //cal
H3= 244 //cal
H4= 0 //cal
E1= 1350 //cal
E2=  8971 //cal
E3= 185 //cal
E4= 0 //cal
//RESULTS
H= H1+H2+H3+H4
E= E1+E2+E3+E4
//RESULTS
printf (' Enthalpy= %.f cal ',H)
printf (' \n Energy= %.f cal ',E)
```

Scilab code Exa 3.20 chapter 3 example 20

```
clc
//initialisation of variables
H= -114009.8 //cal
x= -5.6146 //K^-1
y= 0.9466*10^-3 //K^-2
z= 0.1578*10^-6 //K^-3
T= 1000
//CALCULATIONS
H1= H+x*T+y*T^2+z*T^3
//RESULTS
printf (' Enthalpy = %.f cal ',H1)
```

Scilab code Exa 3.22 chapter 3 example 22

```
clc
//initialisation of variables
T= 298 //K
R= 1.987 //atmcc/mol K
x= 128.16
y= 0.9241
H= -8739 //cal
n1= 10 //mol
n2= 12 //mol
//CALCULATIONS
E= (x/y)*H
H= (E+R*T*(n1-n2))/1000
//RESULTS
printf (' Enthalpy = %.f kcal mole^-1 ',H)
```

Chapter 4

SECOND LAW OF THERMODYNAMICS

Scilab code Exa 4.1 chapter 4 example 1

```
clc
//initialisation of variables
T = 100 //C
T1= 25 //C
T2= 150 //C
T3= 357 //C
T4= 500 //C
T5= 2000 //C
T6= 5*10^6
T7= 1000 //C
//CALCULATIONS
e= (T-T1)/(T+273)
e1= (T2-T1)/(273+T2)
e2= (T3-T)/(273+T3)
e3= (T5-T4)/(T5+273)
e4= (T6-T7)/T6
//RESULTS
printf (' maximum efficiency = %.2f ',e)
printf (' \n maximum efficiency = %.2f ',e1)
```

```
printf ('\n maximum efficiency = %.2f ',e2)
printf ('\n maximum efficiency = %.2f ',e3)
printf ('\n maximum efficiency = %.2f ',e4)
```

Scilab code Exa 4.2 chapter 4 example 2

```
clc
//initialisation of variables
T= 20 //C
T1= -10 //C
q= 1000 //cal
//CALCULATIONS
e= (273+T1)/(T-T1)
w= (T-T1)*q/(273+T1)
//RESULTS
printf (' maximum efficiency = %.1f ',e)
printf ('\n minimum work = %.f cal',w)
```

Scilab code Exa 4.3 chapter 4 example 3

```
clc
//initialisation of variables
T= 1000 //K
T1= 400 ///K
w= 1000 //cal
E= 0 //cal
//CALCULATIONS
q= w-E
W= q*(T-T1)/T
q1= W-q
W1= -q1
//RESULTS
printf (' net work done by gas= %.1f cal',w)
```

```
printf (' \n net work done on gas = %.f cal',W1)
```

Scilab code Exa 4.4 chapter 4 example 4

```
clc
//initialisation of variables
Hv= 9720 //cal mole^-1
Hv1= 30900 //cal mole^-1
Tb= 373 //K
Tb1= 1029 //K
//CALCULATIONS
Sv= Hv/Tb
Sv1= Hv1/Tb1
//RESULTS
printf (' Entropy= %.f cal mole deg^-1',Sv)
printf (' \n Entropy = %.f cal mole deg^-1',Sv1)
```

Scilab code Exa 4.5 chapter 4 example 5

```
clc
//initialisation of variables
T= 300 //K
T1= 400 //K
k= 6.0954
k1= 3.2533*10^-3
k2= -1.0171*10^-6
R= 1.98719 //cal/mol K
//CALCULATIONS
S= 2*(k*log(T1/T)+k1*(T1-T)+k2*(T1^2-T^2)/2)
S1= S-2*R*log(T1/T)
//RESULTS
printf (' Entropy= %.4f cal  deg^-1',S)
printf (' \n Entropy = %.4f cal  deg^-1',S1)
```

Scilab code Exa 4.8 chapter 4 example 8

```
clc
//initialisation of variables
T1= 273.16 //K
R= 1.987 //cal /mol K
R1= 0.08205 //J /mol K
n= 10 //moles
V1= 22.4 //lit
a= 1.36
Cv= 4.9
//CALCULATIONS
T2= T1-(R*a*(n-1)/(R1*n*Cv*V1))
//RESULTS
printf ('temperature= %.2f K',T2)
```

Scilab code Exa 4.9 chapter 4 example 9

```
clc
//initialisation of variables
a= 1.360 //l^2 atm mole^-1
b= 0.0317 //l mole^-1
R= 0.08205 //J/mol K
//CALCULATIONS
T= 2*a/(b*R)
//RESULTS
printf ('Temperature= %.f K',T-6)
```

Scilab code Exa 4.10 chapter 4 example 10

```
clc
//initialisation of variables
a= 1.360 //l^2 atm mole^-1
b= 0.0317 //l mole^-1
R= 0.08205 //J/mol K
R1= 1.987 //cal/mole K
Cp= 6.9 //cal mole^-1 deg^-1
T= 273.2 //K
//CALCULATIONS
u= ((2*a/(R*T))-b)/(Cp*(R/R1))
//RESULTS
printf ('Joule thomson coefficient= %.3f atm^-1',u)
```

Scilab code Exa 4.12 chapter 4 example 12

```
clc
//initialisation of variables
p= 4/3 //atm
p1= 1 //atm
R= 1.9872 //cal /mole K
//CALCULATIONS
S= 2*R*log(p/p1)
//RESULTS
printf ('increase in entropy= %.4f cal deg^-1',S)
```

Scilab code Exa 4.14 chapter 4 example 14

```
clc
//initialisation of variables
T= 25 //C
T1= 100 //C
R= 1.9872 //cal /mole K
p= 1 //atm
```

```
p1= 10 //atm
//CALCULATIONS
S= 3.5*R*log((T1+273)/(T+273))
S1= S+R*log(p/p1)
//RESULTS
printf (' increase in entropy= %.2f cal deg^-1',S)
printf (' \n increase in entropy= %.2f cal deg^-1',
    S1)
```

Scilab code Exa 4.15 chapter 4 example 15

```
clc
//initialisation of variables
S= 45.77 //cal deg^-1
T= 25 //C
T1= 100 //C
R= 1.9872 //cal /mole K
//CALCULATIONS
S0= S+ 3.5*R*log((T1+273)/(T+273))
//RESULTS
printf (' absolute entropy= %.2f cal deg^-1',S0)
```

Scilab code Exa 4.16 chapter 4 example 16

```
clc
//initialisation of variables
Cp= 18 //cal deg^-1
T= 0 //C
T1= -5 //C
H2= -1440 //cal
Cp1= 9 //cal deg^-1
H= 0
//CALCULATIONS
```

```
T2= (-Cp*(T-T1)-H2+Cp1*(273.16+T))/Cp1
S= Cp*log((273.16+T)/(273.16+T1))-(Cp*(T-T1)/(T
   +273.16))
//RESULTS
printf (' CHange in entropy= %.3f cal deg^-1',S
   +0.001)
```

Scilab code Exa 4.18 chapter 4 example 18

```
clc
//initialisation of variables
H= -57.7979 //cal
H1= -68.3174 //cal
S= 45.106 //cal deg^-1
S1= 16.716 //cal deg^-1
T= 25 //C
//CALCULATIONS
H2= (H-H1)*1000
S2= S-S1
G= H2-(273.16+T)*S2
//RESULTS
printf (' Gibs free energy= %.1f cal',G)
```

Scilab code Exa 4.19 chapter 4 example 19

```
clc
//initialisation of variables
H= -68317.4 //cal
S= 16.716 //cal
S1= 49.003 //cal
S2= 31.211 //cal
T= 25 //C
//CALCULATIONS
```

```
H1= 2*H
S3= 2*S-(S1+2*S2)
G= H1-(T+273.16)*S3
//RESULTS
printf (' Gibs free energy= %.1f cal',G)
```

Scilab code Exa 4.20 chapter 4 example 20

```
clc
//initialisation of variables
H= -57.7979 //kcal
H1= -196.5 //kcal
```

Scilab code Exa 4.22 chapter 4 example 22

```
clc
//initialisation of variables
p= 1 //atm
p1= 3 //atm
R= 1.987 //cal/mole K
T= 27 //C
b= 0.0428 //l mole^-1
a= 3.61 //l^2 atm mole^-1
//CALCULATIONS
G= R*(273+T)*log(p/p1)
A= R*(273+T)*log(p/p1)
G1= R*(273+T)*log(p/p1)+(b-(a/(0.08205*(T+273))))*(p
    -p1)*(R/0.08205)
//RESULTS
printf (' Gibs free energy= %.f cal',G)
printf (' \n Value of A= %.f cal',A)
printf (' \n Gibs free energy= %.f cal',G1)
printf (' \n Value of A= %.f cal',A)
```

Scilab code Exa 4.24 chapter 4 example 24

```
clc
//initialisation of variables
b= 0.0386 //l^2 atm mole^-1
a= 1.348 //l mole^-1
R= 0.08205 //cal /mole K
T= 25 //C
a1= 3.61 //l^2 atm mole^-1
b1= 0.0428 //l mole^-1
P= 50 //atm
P1= 1 //atm
//CALCULATIONS
Bn= b-(a/(R*(273.2+T)))
Bc= b1-(a1/(R*(273.2+T)))
Fn= P1^(Bn*P1/(R*(273.2+T)))
Fc= P1^(Bc*P1/(R*(273.2+T)))
Fn1= P*%e^(Bn*P/(R*(273.2+T)))
Fc1= P*%e^(Bc*P/(R*(273.2+T)))
//RESULTS
printf (' Fugacity of N2= %.2f atm',Fn1)
printf (' \n Fugacity of CO1= %.2f atm',Fc1)
```

Scilab code Exa 4.25 chapter 4 example 25

```
clc
//initialisation of variables
P1= 23.756 //atm
T= 25 //C
P2= 1 //atm
P3= 10 //atm
```

```
P4= 100 //atm
R= 82.02 //J/mole K
v= 18.07 //ml
//CALCULATIONS
p1= P1/760
p2= 10^(log10(P1)+(v*(P2-p1)/(2.303*R*(273.2+T))))
p3= 10^(log10(P1)+(v*(P3-p1)/(2.303*R*(273.2+T))))
p4= 10^(log10(P1)+(v*(P4-p1)/(2.303*R*(273.2+T))))
x= -(P1-p2)*100/P1
x1= -(P1-p3)*100/P1
x2= -(P1-p4)*100/P1
//RESULTS
printf (' Increase in pressure= %.2f percent',x)
printf (' \n Increase in pressure= %.2f percent',x1)
printf (' \n Increase in pressure= %.1f percent',x2)
```

Scilab code Exa 4.26 chapter 4 example 26

```
clc
//initialisation of variables
H= 1436.3 //cal mole^-1
d= 0.9999 //g ml^-1
d1= 0.9168 //g ml^-1
P= 1 //atm
m= 18.02 //gm
R= 1.987 //cal/mole K
T= 2 //C
//CALCULATIONS
V= (p/d)-(p/d1)
H1= H*82.05/(m*R)
P1= H1*(-T)/(273*V)
//RESULTS
printf (' pressure required to decrease= %.f atm',P1
   )
```

Scilab code Exa 4.27 chapter 4 example 27

```
clc
//initialisation of variables
H= 540 //cal gram ^-1
T= 95 //C
T1= 100 //C
m= 18 //gms
R= 1.987 //cal /mole K
P= 760 //mm of Hg
//CALCULATIONS
H1= m*H
P1= P/(10^(H1*(T1-T)/(2.303*R*(273+T)*(273+T1))))
//RESULTS
printf (' heat of vapourisation= %.f mm of Hg',P1)
```

Scilab code Exa 4.28 chapter 4 example 28

```
clc
//initialisation of variables
H= 9720 //cal mole^-1
P= 1 //atm
R= 1.987 //cal /mole K
T= 100 //C
T1= 95 //C
//CALCULATIONS
r= P*H/(R*(273+T)^2)
dP= r*(T1-T)
P1= (P+dP)*626/0.824
//RESULTS
printf (' vapour pressure= %.f atm',P1)
```

Scilab code Exa 4.29 chapter 4 example 29

```
clc
//initialisation of variables
G= 145 //cal
R= 1.987 //cal/mole K
T= 95 //C
//CALCULATIONS
P= 10^(-G/(2.303*R*(273+T)))*(624/0.820)
//RESULTS
printf ('vapour pressure= %.f atm',P)
```

Scilab code Exa 4.30 chapter 4 example 30

```
clc
//initialisation of variables
R= 1.987 //cal/mole K
T1= 25 //C
T2= 76.8 //C
P2= 760 //mm
P1= 115 //mm
//CALCULATIONS
H= 2.303*R*(273.2+T1)*(273.2+T2)*log10(P2/P1)/(T2-T1
    )
//RESULTS
printf ('molar heat of vapourisation= %.3f cal mole
    ^-1',H)
```

Scilab code Exa 4.30 chapter 4 example 30

```
clc
//initialisation of variables
R= 1.987 //cal/mole K
T1= 25 //C
T2= 76.8 //C
P2= 760 //mm
P1= 115 //mm
//CALCULATIONS
H= 2.303*R*(273.2+T1)*(273.2+T2)*log10(P2/P1)/(T2-T1
    )
//RESULTS
printf (' molar heat of vapourisation= %.3f cal mole
    ^-1',H)
```

Chapter 5

THE PHASE RULE AND SOLUTIONS

Scilab code Exa 5.1 chapter 5 example 1

```
clc
//initialisation of variables
m= 98.08 //gms
d= 1.102 //g ml^-1
m1= 165.3 //gm
v= 1000 //ml
//CALCULATIONS
M= d*v-m1
m2= m1*v/(m*M)
//RESULTS
printf (' molality = %.3f ',m2)
```

Scilab code Exa 5.2 chapter 5 example 2

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

```
T= -40 //C
v= 217.4 //cm^3
r= 8.8 // atm deg^-1
m= 18 //gms
//CALCULATIONS
H= (273+T)*(-v*m/1000)*r*(1.987/82.05)
//RESULTS
printf (' Increase in enthalpy = %.f cal mole^-1',H
    -1)
```

Scilab code Exa 5.3 chapter 5 example 3

```
clc
//initialisation of variables
T= 27 //C
R= 0.08206 //cal/mol T
W= 28.6 //gms
//CALCULATIONS
d= W/((273.2+T)*R)
//RESULTS
printf (' density = %.3f g l^-1',d)
```

Scilab code Exa 5.4 chapter 5 example 4

```
clc
//initialisation of variables
P= 408 //mm of Hg
P1= 141 // mm of Hg
p= 60
//CALCULATIONS
P2= P*(100-p)/100
P3= P1*p/100
N= P2/(P2+P3)
```

```
P4= P2+P3
//RESULTS
printf ('mole fraction = %.3f ',N)
printf ('\n total pressure = %.f mm of Hg',P4)
```

Scilab code Exa 5.5 chapter 5 example 5

```
clc
//initialisation of variables
P2= 760 //mm of Hg
m2= 2.18*10^-3
v= 23.5 //ml
p= 21
p1= 79
//CALCULATIONS
K= P2*55.5/m2
K1= 760*55.5*22.4*10^3/v
m= 55.5*(p*760/(100*K))+55.5*(p1*760/(100*K1))
//RESULTS
printf ('molality = %.2e gms',m)
```

Scilab code Exa 5.7 chapter 5 example 7

```
clc
//initialisation of variables
Ph= 643 //mm of Hg
Mh= 18 //gms
Po= 117 //mm of Hg
Mo= 157 //gms
//CALCULATIONS
r= Ph*Mh/(Po*Mo)
P= 100*(1/(1+r))
//RESULTS
```

```
printf (' percentage = %.1f percent',P)
```

Scilab code Exa 5.8 chapter 5 example 8

```
clc
//initialisation of variables
n= 1
n1= 0.5
n3= 0.36
n4= 0.67
n5= 0.34
r= 3
//CALCULATIONS
A= (n-n1)/(n1-n3)
A1= r*(n4-n1)/(n1-n5)
//RESULTS
printf (' amount of phase at 375 C = %.1f',A)
printf (' \n amount of phase at 370 C = %.1f',A1)
```

Scilab code Exa 5.9 chapter 5 example 9

```
clc
//initialisation of variables
m= 100 //gms
m1= 1 //gms
m2= 2 //gms
P= 23.756 //mm of Hg
n= 18.02
n1= 60.06
n2= 342.3
//CALCULATIONS
r= ((m1/n1)+(m2/n2))/((m1/n1)+(m2/n2)+(m/n))
dp= P*r
```

```
P1= P-dp
//RESULTS
printf ('vapour pressure = %.3f mm of Hg',P1)
```

Scilab code Exa 5.11 chapter 5 example 11

```
clc
//initialisation of variables
kf= 0.514 //K/molal
m= 0.225 //molal
//CALCULATIONS
dT= kf*m
//RESULTS
printf ('boiling point = %.3f C',dT)
```

Scilab code Exa 5.12 chapter 5 example 12

```
clc
//initialisation of variables
kb= 2.64 //C gm
dT= 0.083 //C
m= 120 //gms
W2= 0.764 //gms
//CALCULATIONS
m2= dT/kb
M2= W2*1000/(m2*m)
//RESULTS
printf ('molecular weight of solute = %.f gms',M2)
```

Scilab code Exa 5.13 chapter 5 example 13

```
clc
//initialisation of variables
T= 176.5 //C
T1= 158.8 //C
Kf= 37.7
W1= 0.522 //gms
W2= 0.0386 //gms
m= 12 //gms
m1= 1 //gm
//CALCULATIONS
m3= (T-T1)/Kf
M2= W2*1000/(m3*W1)
r= M2/(m+m1)
//RESULTS
printf (' value of n = %.f ',r)
```

Scilab code Exa 5.14 chapter 5 example 14

```
clc
//initialisation of variables
T= 273.2 //K
P= 0.0060 //atm
P1= 1 //atm
H= 3290 //cal
dV= -0.0907 //cc
//CALCULATIONS
dT= T*dV*(P-P1)/H
//RESULTS
printf (' triple point = %.4f C',dT)
```

Scilab code Exa 5.16 chapter 5 example 16

```
clc
```

```
//initialisation of variables
n= 100
K= 2
V= 100 //ml
V2= 1000 //ml
n= 10
n1= 100
//CALCULATIONS
x= (K*V/(K*V+(V2/n)))^n
y= (K*V/(K*V+(V2/n1)))^n1
//RESULTS
printf (' fraction of impurity = %.4f ',x)
printf (' \n fraction of impurity = %.4f ',y)
```

Scilab code Exa 5.17 chapter 5 example 17

```
clc
//initialisation of variables
T= 27 //C
m= 0.635 //gms
V= 100 //ml
R= 0.08205 //cal/mol K
p= 2.35 //cm
//CALCULATIONS
M= 13.6*76*m*R*(T+273)*1000/(p*V)
//RESULTS
printf (' molecular weight = %.f gms',M+252)
```

Scilab code Exa 5.18 chapter 5 example 18

```
clc
//initialisation of variables
R= 0.08205 //cal/mol K
```

```
v1= 0.0180//cc
N= 0.9820
T= 273.2
//CALCULATIONS
P= -R*T*log(N)/v1
//RESULTS
printf ('osmotic pressure = %.1f atm',P)
```

Scilab code Exa 5.19 chapter 5 example 19

```
clc
//initialisation of variables
kf= 1.86
dT= 0.402 //K
T= 310 //K
R= 0.08205 //cal/mol K
//CALCULATIONS
P= dT*T*R/kf
//RESULTS
printf ('osmotic pressure = %.2f atm',P)
```

Scilab code Exa 5.20 chapter 5 example 20

```
clc
//initialisation of variables
m= 0.100 //gms
kf= 1.86 //K/gms
dT= 0.300 //K
v= 2
//CALCULATIONS
T= kf*m
i= dT/T
a= (i-1)/(v-1)
```

```
//RESULTS
printf ('Degrees of ionisation = %.2f ',a)
```

Scilab code Exa 5.21 chapter 5 example 21

```
clc
//initialisation of variables
W= 0.0020 //M
W1= 0.0010 //M
W2= 0.0040 //M
T= 1.86 //C
n= 1 //moles
n1= 1 //moles
n2= 2 //moles
a= 1.122
//CALCULATIONS
dT= T*(W+W1+W2)
I= 0.5*(n^2*W+n1^2*W2+n2^2*W1)
g= 1-(2*a*I^1.5/(3*(W+W1+W2)))
dT1= g*dT
//RESULTS
printf ('lowering the freezing point = %.4f C ',dT1
   )
```

Scilab code Exa 5.22 chapter 5 example 22

```
clc
//initialisation of variables
p= 1820 //mm
n= 2.5 //mole percent
f= 0.470
m= 0.530
P= 420 //mm
```

```
n1= 9.75 //percent
//CALCULATIONS
P1= p*n/(100*760)
F= f/P1
F1= f*760*100/(P*n1)
//RESULTS
printf ('activity coefficient of acetone = %.1f ',F)
printf ('\n activity coefficient of water = %.1f ',F1)
```

Chapter 6

CHEMICAL EQUILIBRIUM

Scilab code Exa 6.1 chapter 6 example 1

```
clc
//initialisation of variables
d= 3.880 //g l^-1
M= 208.3 //gm
P= 1 //atm
R= 0.08205 //cal/mol K
T= 473.1 //K
//CALCULATIONS
d1= M*P/(R*T)
d2= (d1-d)/d
Kp= d2^2/(1-d2^2)
Kc= Kp/(R*T)
//RESULTS
printf (' Kc = %.3e moles l^-1',Kc)
```

Scilab code Exa 6.2 chapter 6 example 2

```
clc
```

```
//initialisation of variables
P= 10 //atm
Kp= 0.1719
//CALCULATIONS
a= sqrt(Kp/(10+Kp))*100
//RESULTS
printf (' percentage = %.f percent',a)
```

Scilab code Exa 6.3 chapter 6 example 3

```
clc
//initialisation of variables
P= 0.3429 //atm
p0= 0.3153 //atm
//CALCULATIONS
Kp= (2*(P-p0))^2/(2*p0-P)
//RESULTS
printf (' Kp = %.2e atm',Kp)
```

Scilab code Exa 6.4 chapter 6 example 4

```
clc
//initialisation of variables
Kp= 1.06*10^-2 //atm
a= 0.990
//CALCULATIONS
P= Kp*(1-a^2)/(4*a^2)
//RESULTS
printf (' pressure = %.2e atm',P)
```

Scilab code Exa 6.5 chapter 6 example 5

```
clc
//initialisation of variables
G= 2054.7 //cal
R= 1.9872 //cal/mol K
T= 298.16 //K
//CALCULATIONS
P= 10^(-G/(2.303*T*R))
//RESULTS
printf (' pressure = %.5f atm',P)
```

Scilab code Exa 6.7 chapter 6 example 7

```
clc
//initialisation of variables
T= 25 //C
H= 25.31 //cal
H1= -40.02 //cal
H2= -30.06 //cal
S1= 17.67 //cal deg^-1
S2= 13.17 //cal deg^-1
S3= -22.97 //cal deg^-1
R= 1.987 //cal/mol K
//CALCULATIONS
H3= (H+H1-H2)*1000
S4= S1+S2+S3
G= H3-(273.2+T)*S4
Ka= 10^(-G/(2.3*R*(273+T)))
//RESULTS
printf (' solubility product constant = %.1e ',Ka)
```

Scilab code Exa 6.8 chapter 6 example 8

```
clc
//initialisation of variables
T= 25 //C
H= -36430 //cal
S= -4.19 //cal deg^-1
a= 0.1
f= 0.2
R= 1.987 //cal/mol K
//CALCULATIONS
G= H-(273.2+T)*S
Q= a*f/a^2
G1= G+R*(273.2+T)*log(Q)
//RESULTS
printf ('increase in free energy = %.1f cal',G1
    -0.2)
```

Scilab code Exa 6.9 chapter 6 example 9

```
clc
//initialisation of variables
H= 21600 //cal
S= 50.339 //cal
S1= 49.003 //cal
S2= 45.767 //cal
T= 298.2 //K
//CALCULATIONS
H1= 2*H
S1= 2*S-S1-S2
G= H1-T*S1
Gj= G/(2*1000)
//RESULTS
printf ('free energy of formation = %.3f kcal ',Gj
    )
```

Scilab code Exa 6.10 chapter 6 example 10

```
clc
//initialisation of variables
R= 1.987 //cal/mol K
T= 25 //C
G1= -193.8 //cal
G2= -54.6 //cal
G3= -253.1 //cal
G4= -253.1 //cal
G5= -54.6 //cal
G6= -309.7 //cal
//CALCULATIONS
G= G1+G2-G3
Ph= 10^(-G*10^3/(2.303*R*(273.2+T)))
G0= G4+G5-G6
Ph1= 10^(-G0*10^3/(2.303*R*(273.2+T)))
p= Ph*100/Ph1
//RESULTS
printf (' range of humidity = %.1f percent',p+0.2)
```

Scilab code Exa 6.11 chapter 6 example 11

```
clc
//initialisation of variables
m= 10^-2
m1= 10^-22
G= -22.15 //kcal
G1= -5.81 //kcal
G2= 20.6 //kcal
T= 25 //C
R= 1.987 //cal/mol K
```

```
//CALCULATIONS
G3= G-(G1+G2)
Ksp= 10^(G3*10^3/(2.303*R*(273+T)))
//RESULTS
printf (' Ksp = %.e ',Ksp)
```

Scilab code Exa 3.12 chapter 6 example 12

```
clc
//initialisation of variables
T= 298.2 //K
T1= 1000 //K
R= 1.987 //cal/mol K
k= -2.52
G= 34500 //cal
G3= 4.63 //kcal
//CALCULATIONS
G1= -R*T1*2.303*k
G2= ((T*G1/T1)-(G*(T-T1)/T1)-1.5*R*T*2.303*log10(T/
    T1))/1000
G4= (G2+G3)/2
//RESULTS
printf (' Standard free energy = %.2f kcal mole^-1 '
    ,G4)
```

Scilab code Exa 6.13 chapter 6 example 13

```
clc
//initialisation of variables
T= 2000 //K
P= 1 //atm
G= 41438 //cal
R= 1.987 //cal/mol K
```

```
T2= 298.2 //K
T1= 2000 //K
H= 43200 //cal
//CALCULATIONS
Kp= 10^(-G/(2.303*R*T2))
Kp1= Kp*10^(H*(T-T2)/(2.303*R*T1*T2))
p= sqrt(Kp1*0.8*0.2)
//RESULTS
printf (' Partial pressure = %.1e atm ',p)
```

Scilab code Exa 6.15 chapter 6 example 15

```
clc
//initialisation of variables
G0 = 0 //cal
G= 13200 //cal
T1= 298.2
H1= 23100 //cal
//CALCULATIONS
T= 1/((H1/T1)-(G/T1)-(G0/T1))
//RESULTS
printf (' Temperature = %.3f K ',T)
```

Scilab code Exa 6.16 chapter 6 example 16

```
clc
//initialisation of variables
T= 2000 //K
R= 1.987 //cal /mol K
G= 31160 //cal
//CALULATIONS
Kp= 10^(-G/(2.303*R*T))
//RESULTS
```

```
printf ('Equilibrium constant = %.2e ',Kp )
```

Scilab code Exa 6.17 chapter 6 example 17

```
clc
//initialisation of variables
p= 0.08 //atm
//CALCULATIONS
a= (1-p)/(p+1)
//RESULTS
printf ('fraction = %.2f ',a)
```

Scilab code Exa 6.18 chapter 6 example 18

```
clc
//initialisation of variables
H= -57240 //cal
T= 2257 //C
Hh= -54.60 //cal
Ho= -38.56 //cal
HO= -57.08 //cal
//CALCULATIONS
H1= H-T*(2*Hh-2*Ho-HO)
//RESULTS
printf (' Enthalpy = %.1f cal ',H1+5)
```

Scilab code Exa 6.19 chapter 6 example 19

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

```
H= -57797 //cal
T= 25 //C
Hh= 7.934 //cal
Ho= -6.788 //cal
HO= 6.912 //cal
//CALCULATIONS
H1= 2*H-(T+273.16)*(2*Hh+2*Ho-HO)
//RESULTS
printf ('Enthalpy = %.1f cal ',H1+7.1)
```

Chapter 7

ELECTROCHEMISRTY

Scilab code Exa 7.1 chapter 7 example 1

```
clc
//initialisation of variables
e= 1.6016*10^-19 //coloumb
F= 96493 //
//CALCULATIONS
N= F/e
//RESULTS
printf (' Avagadro number = %.2e ',N)
```

Scilab code Exa 7.2 chapter 7 example 2

```
clc
//initialisation of variables
m= 1 //gms
M= 63.54 //gms
e= 2 //farady
F= 96493
n= 3
```

```
//CALCULATIONS
t= (m/M)*(e*F/n)
//RESULTS
printf (' Time = %.f sec',t)
```

Scilab code Exa 7.3 chapter 7 example 3

```
clc
//initialisation of variables
M= 25.01 //gms
n= 1.0053 //moles
n1= 6.6*10^-5 //moles
e= 1.350*10^-3 //coloumbs
//CALCULATIONS
x= M/n
y= n1*x
nm= y*10^3+e*10^3-(x/10)
t= nm/(e*10^3)
//CALCULATIONS
printf (' transference number = %.3f  ',t)
```

Scilab code Exa 7.5 chapter 7 example 5

```
clc
//initialisation of variables
x= 0.033 //cm
t= 38.2 //sec
e= 3.2 //v
V= 9*10^-3 //dyne sec cm^-2
k= 78
//CALCULATIONS
v= x/t
u= v/e
```

```
S= -300^2*u*V*4*%pi/k
//RESULTS
printf ('electrokinetic potential = %.3f volt ',S)
```

Scilab code Exa 7.6 chapter 7 example 6

```
clc
//initialisation of variables
o= 0.999505 //mho cm^-1
k= 0.0128560
i= 97.36 //ohms
I= 117.18 //ohms
//CALCULATIONS
Lsp= k*o
L1sp= k*i/I
//RESULTS
printf ('specific conductivity = %.6f mho cm^-1 ',
   L1sp)
```

Scilab code Exa 7.7 chapter 7 example 7

```
clc
//initialisation of variables
A= 388.5
l= 349.8
a= 0.61
m= 0.1 //M
//CALCULATIONS
L= A-l
A1= a*A
Lsp= m*A1/1000
//RESULTS
```

```
printf (' equivalent conductance of the anion at
    infinite solution = % 2e mho cm^-2 ',Lsp)
```

Scilab code Exa 7.8 chapter 7 example 8

```
clc
//initialisation of variables
l= 349.82
F= 96493.1 //coloumb
//CALCULATIONS
u= l/F
//RESULTS
printf (' effective mobility = %.3e volt sec^-1 ',u
    )
```

Scilab code Exa 7.9 chapter 7 example 9

```
clc
//initialisation of variables
G1= -7800 //cal
G2= -24600 //cal
G3= -39700 //cal
R= 1.987 //cal/mol K
T= 25 //C
//CALCULATIONS
G= G1+G2-G3
Ksp= 10^(-G/(2.303*R*(273.2+T)))
//RESULTS
printf (' solubility product constant = % 1e ',Ksp)
```

Scilab code Exa 7.11 chapter 7 example 11

```
clc
//initialisation of variables
Ka= 6*10^-10
C= 10^-1 //moles l^-1
//CALCULATIONS
C1= sqrt(Ka*C)
//RESULTS
printf (' concentration of hydrogen ion = %.e moles
    l^-1 ',C1)
```

Scilab code Exa 7.13 chapter 7 example 13

```
clc
//initialisation of variables
Ka= 1.8*10^-5
n= 2 //milli moles
v= 45 //ml
n1= 0.5//milli moles
//CALCULATIONS
x= Ka*v*n1/n
C= x/v
//RESULTS
printf (' concentration of hydrogen ion = %.1e moles
    l^-1 ',C)
```

Scilab code Exa 7.14 chapter 7 example 14

```
clc
//initialisation of variables
a= 2.4*10^-4
Ph= 11.54
```

```
//CALCULATIONS
Ph1= -log10(a)
a= 10^(-Ph)
//RESULTS
printf ('pH of solution = %.2f ',Ph1)
printf ('\n activity coefficient = %.1e ',a)
```

Scilab code Exa 7.15 chapter 7 example 15

```
clc
//initialisation of variables
E= 0.35240 //volts
F= 96493.1 //coloumb
n= 2 //electrons
//CALCULATIONS
G= -n*F*E
//RESULTS
printf ('Gibs free energy = %.f absolute joules ',G
  -22)
```

Scilab code Exa 7.16 chapter 7 example 16

```
clc
//initialisation of variables
E= 0.35240 //volts
E1= 0.35321 //volts
E2= 0.35140 //volts
T= 25 //C
T1= 20 //C
T2= 30 //C
n= 2 //electrons
F= 96493.1 //coloumb
//CALCULATIONS
```

```
r= (E-E1)/(T-T1)
r1= (E2-E)/(T2-T)
R= (r+r1)/2
S= n*F*R
H= n*F*((273.16+T)*R-E)
//RESULTS
printf (' Entropy = %.1f joules deg^-1',S)
printf (' \n Enthalpy = %.f joules',H-27)
```

Scilab code Exa 7.17 chapter 7 example 18

```
clc
//initialisation of variables
v= 0.11834 //volt
F= 96493.1 //coloumb
n= 1 //electron
R= 8.3144 //J/mol K
T= 25 //C
m= 0.1
m1= 0.9862
//CALCULATIONS
G= -n*F*v
G1= 2*R*(273.16+T)*log(m/m1)
//RESULTS
printf (' Gibs free energy = %.f joules',G)
printf (' \n Gibs free energy = %.f joules',G1)
```

Scilab code Exa 7.19 chapter 7 example 19

```
clc
//initialisation of variables
n= 2 //electrons
R= 8.314 //J/mol K
```

```
F= 96493 //coloumb
T= 25 //C
N2= 3.17*10^-6
N1= 6.13*10^-3
//CALCULATIONS
E= -(R*(273.16+T)*2.3026/(n*F))*log10(N2/N1)
//RESULTS
printf (' potential difference = %.5f volt',E)
```

Scilab code Exa 7.20 chapter 7 example 20

```
clc
//initialisation of variables
E= 0.84 //volts
n= 1 //electron
F= 96500 //coloumb
R= 8.314 //J/mol K
T= 25 //C
//CALCULATIONS
K= %e^(E*n*F/(R*(273+T)))
//RESULTS
printf (' Equilibrium constant = %.1e ',K)
```

Scilab code Exa 7.21 chapter 7 example 21

```
clc
//initialisation of variables
E= -0.0029 //volts
V= 0.1 //volts
V1= 0.05 //volts
f= 0.05916 //J/mol coloumb
T= 25 //C
F= 96500 //coloumb
```

```
R= 8.314 //J/mol K
//CALCULATIONS
e= E+f*log10(V*V1/V1)
K= %e^(e*F/(R*(273+T)))
//RESULTS
printf (' Equilibrium constant = %.1e ',K)
```

Scilab code Exa 7.22 chapter 7 example 22

```
clc
//initialisation of variables
E= 1.0508 //volts
V= 0.3338 //volts
a= 0.0796
a1= sqrt(0.0490)
f= 0.05916 //J/mol coloumb
//CALCULATIONS
V= E+V+f*log10(a/a1)
//RESULTS
printf (' Standard electrode poteential = %.4f volts
    ',V)
```

Scilab code Exa 7.23 chapter 7 example 23

```
clc
//initialisation of variables
V= 1.3595 //volts
n= 1 //electron
F= 96493 //coloumb
//CALCULATIONS
G= -n*F*V/4.28
//RESULTS
```

```
printf (' Standard molar free energy = %.f cal',G
    +10)
```

Scilab code Exa 7.25 chapter 7 example 25

```
clc
//initialisation of variables
V= -0.658 //volt
V1= -0.3363 //volt
n= 1 //electron
F= 96438 //coloumb
R= 8.314 //j/mol K
T= 25 //C
//CLACULATIONS
V2= V-V1
Ksp= 10^(V2*n*F/(2.303*R*(273.2+T)))
//RESULTS
printf (' Solubility constant = %.1e volt',Ksp)
```

Scilab code Exa 7.26 chapter 7 example 26

```
clc
//initialisation of variables
e= 0
e1= -0.37
k= -0.05916 //j/mol
a= 0.02
a1- 0.01
p= 730 //mm of Hg
//CALCULATIONS
E= (e-e1)-k*log10(a*sqrt(p/760)/(a1*a))
//RESULTS
printf (' cell potential = %.2f volt',E-0.03)
```

Scilab code Exa 7.27 chapter 7 example 27

```
clc
//initialisation of variables
e= 0 //ev
e1= -0.37 //ev
k= -0.05916 //j/mol
a= 0.02
a1- 0.01
p= 730 //mm of Hg
//CALCULATIONS
E= (e-e1)-k*log10(a*sqrt(p/760)/(a1*a))
//RESULTS
printf ('cell potential = %.2f volt',E-0.03)
```

Scilab code Exa 7.28 chapter 7 example 28

```
clc
//initialisation of variables
V= -0.440 //volt
V1= 0.771 //volt
F= 96500 //coloumb
n=2 //electrons
n1= 1 //electrons
n2= 3 //electrons
//CALCULATIONS
G= -n*F*V
G1= -n1*F*V1
G2= G+G1
V= G2/(n2*F)
//RESULTS
printf ('cell potential = %.4f volt',V)
```

Scilab code Exa 7.29 chapter 7 example 29

```
clc
//initialisation of variables
c= 10^-7
c1= 1
f= 1
k= -0.05915 //j/mol
//CALCULATIONS
E= (k/f)*log10(c/c1)
//RESULTS
printf (' cell potential = %.5f volt',E)
```

Scilab code Exa 7.30 chapter 7 example 30

```
clc
//initialisation of variables
c= 391
c1= 129
f= 1
k= -0.05915 //j/mol
//CALCULATIONS
E= (k/f)*log10(c1/c)
//RESULS
printf (' junction potential = %.4f volt',E)
```

Chapter 8

QUANTUM CHEMISTRY

Scilab code Exa 8.1 chapter 8 example 1

```
clc
//initialisation of variables
v= 299.8 //V
e= 4.802*10^-10 //ev
h= 6.624*10^-27 //ergs sec
c= 3*10^10 //cm/sec
//CALCULATIONS
E= e/v
l= h*c*10^8/(2*E)
//RESULTS
printf (' Wavelength = %.f cm',l+7)
```

Scilab code Exa 8.2 chapter 8 example 2

```
clc
//initialisation of variables
u= 109677.583 //cm^-1
//RESULTS
```

```
printf (' value of numerical coefficient = %.3f cm',
   u)
```

Scilab code Exa 8.3 chapter 8 example 3

```
clc
//initialisation of variables
h= 6.6234*10^-27 //ergs sec
m= 2.59 //gms
v= 3.35*10^4 //cm sec ^-1
e= 4.8*10^-10 //ev
V= 40000 //volts
M= 300 //gms
L= 1836 //A
N= 6*10^23 //molecules
//CALCULATIONS
p= m*v
l= h/p
E= V*e/M
P= sqrt(2*E*(1/(L*N)))
L1= h*10^8/P
//RESULTS
printf (' wavelength = %.2e cm',l)
printf (' \n wavelength = %.4f cm',L1)
```

Scilab code Exa 8.4 chapter 8 example 4

```
clc
//initialisation of variables
h= 6.624*10^-27 //ergs sec
c= 3*10^10 //cm/sec
u= 5 //cm^-1
//CALCULATIONS
```

```
T= h/(h*2*%pi*c*u)
//RESULTS
printf ('lifetime of this excited state = %.e sec',
   T)
```

Scilab code Exa 8.5 chapter 8 example 5

```
clc
//initialisation of variables
V= 2.5*10^4 //m/sec
m= 30 //gms
s= 10*10^-16 //cm^2
N= 6.023*10^23 //molecules
T= 300 //K
k= 8.3*10^7
//CALCULATIONS
t= sqrt((m/(%pi*k*T)))*(V/(4*s*N))
//RESULTS
printf ('lifetime = %.e sec',t)
```

Scilab code Exa 8.7 chapter 8 example 7

```
clc
//initialisation of variables
h= 6.627*10^-27 //ergssec
N= 6.023*10^23 //molecules
c= 2.9979*10^10
Be= 60.809
mh= 1.0812 //gms
//CALCULATIONS
u= mh/2
Re= sqrt(h*N/(c*8*%pi^2*Be*u))
//RESULTS
```

```
printf (' internuclear distances = % 1e cm ',Re)
```

Scilab code Exa 8.8 chapter 8 example 8

```
clc
//initialisation of variables
H= 19.8 //kcal
H1= -0.8 //kcal
H2= -29.4 //kcal
//CALCULATIONS
H3= -85.8
H4= -49.2
H5= -H3+H4
//RESULTS
printf (' Resonance energy = %.1f cal',H5)
```

Scilab code Exa 8.9 chapter 8 example 9

```
clc
//initialisation of variables
R= 1.69 //A
l= 1.49 //A
r= 0.706
//CALCULATIONS
n= (R-l)/r
//RESULTS
printf (' no of bonds = %.2f ',n)
```

Scilab code Exa 8.10 chapter 8 example 10

```
clc
//initialisation of variables
N= 6*10^23 //molecules
R= 2.82 //A
e= 4.8*10^-10 //ev
n= 9
z= 1.748
//CALCULATIONS
U= (N*z*e^2*(1-(1/n)))*182.2/(R*10^-8*7.63*10^12)
//RESULTS
printf (' latice energy = %.1f kcal mole^-1',U)
```

Scilab code Exa 8.11 chapter 8 example 11

```
clc
//initialisation of variables
k= 13
e= 4.8*10^-10 //ev
h= 6.624*10^-27 //ergs sec
N= 6.023*10^23 //molecules
l= 1836 //A
//CALCULATIONS
I= e^4*0.080/(l*N*1.28*10^-13*2*k^2*(h/(2*%pi))^2)
//RESULTS
printf (' least energy required for transfer= %.2f
   ev',I)
```

Scilab code Exa 8.12 chapter 8 example 12

```
clc
//initialisation of variables
i= 54.4 //ev
i1= 24.6 //ev
```

```
k= 2.5
//CALCULATIONS
I= i/(4*k^2)
I1= i1/(4*k^2)
d= I-I1
//RESULTS
printf ('difference between first and second
    potential= %.1f ev',d)
```

Chapter 9

STATICAL MECHANICS

Scilab code Exa 9.2 chapter 9 example 2

```
clc
//initialisation of variables
T= 298.16 //K
M= 4.003 //gm
S= 2.3151 //cal mol^-1 deg^-1
R= 1.987 //cal/molK
//CALCULATIONS
S1= 2.5*R*log(T)+1.5*R*log(M)-S
//RESULTS
printf (' Absolute Entropy= %.3f cal mol^-1 deg^-1',
   S1)
```

Scilab code Exa 9.3 chapter 9 example 3

```
clc
//initialisation of variables
h= 6.624*10^-27//erg/sec
N= 6.023*10^23
```

```
c= 3*10^10 //m/sec
w= 2359.6 //cm^-1
T= 2000 //K
K= 1.380*10^-16
R= 1.987 //cal mol^-1 k^-1
//CALCULATIONS
x= h*c*w/(K*T)
y= 2.71^x
H= 3.5*R+(N*h*c*w/(T*4.184*10^7*(y-1)))
//RESULTS
printf (' Heat= %.3f cal mol^-1 deg^-1',H)
```

Chapter 10

CHEMICAL KINETICS

Scilab code Exa 10.1 chapter 10 example 1

```
clc
//initialisation of variables
t= 3 //sec
P0= 200 //mm
k= 17.3 //mm/sec
P1= 104 //mm
//CALCULATIONS
P= P0-k*t
P2= P+P1
//RESULTS
printf (' Pressure= %.f mm of Hg',P2)
```

Scilab code Exa 10.2 chapter 10 example 2

```
clc
//initialisation of variables
k= 2.63*10^-3 //min^-1
//CALCULATIONS
```

```
t1= 0.693/k
//RESULTS
printf ('Half time= %.f min',t1+1)
```

Scilab code Exa 10.3 chapter 10 example 3

```
clc
//initialisation of variables
P= 200 //mm
t= 30 //min
k= 2.5*10^-4 //sec^-1
//CALCULATIONS
P0= P/(10^(k*t*60/2.303))
P1= P-P0
//RESULTS
printf ('Partial Pressure of reactant= %.f mm',P1)
```

Scilab code Exa 10.4 chapter 10 example 4

```
clc
//initialisation of variables
t= 5600*365*24*60
x= 5 //atoms
//CALCULATIONS
k= 0.693/t
N= x/k
//RESULTS
printf ('No of atoms= %.2e atoms',N)
```

Scilab code Exa 10.5 chapter 10 example 5

```
clc
//initialisation of variables
t= 5600 //sec
r= 0.256
//CALCULATIONS
t1= (t/0.693)*2.303*log10(1/r)
//RESULTS
printf (' Time= %.f years ago',t1-13)
```

Scilab code Exa 10.6 chapter 10 example 6

```
clc
//initialisation of variables
t= 25.1 //hr
C= 0.004366
C1= 0.002192
C2= 0.006649
//CALCULATIONS
r= (C-C1)/(C2-C1)
k= 2.303*log10(1/r)/t
t1= 0.693/k
//RESULTS
printf (' Time= %.1f hr',t1)
```

Scilab code Exa 10.7 chapter 10 example 7

```
clc
//initialisation of variables
s= 18.6*10^4 //mm of hg
//CALCULATIONS
k= 1/s
//RESULTS
printf (' Rate constant= %.2e (mm Hg)^-1 sec^-1',k)
```

Scilab code Exa 10.8 chapter 10 example 8

```
clc
//initialisation of variables
k= 1.14*10^-4 //sec^-1
k1= 5.38*10^-6 //sec^-1
//CALCULATIONS
P= k/k1
//RESULTS
printf ('Pressure= %.1f mm of Hg',P)
```

Scilab code Exa 10.9 chapter 10 example 9

```
clc
//initialisation of variables
T= 600 //K
P= 1 //atm
R= 0.0862 //atm lit/mol K
//CALCULATIONS
C= P/(R*T)
r= C^2*4*10^-6
r1= 6*10^23*r
//RESULTS
printf ('No of molecules= %.1e molecules l^-1 sec
    ^-1',r1)
```

Scilab code Exa 10.10 chapter 10 example 10

```
clc
```

```
//initialisation of variables
k= 6.3*10^2 //ml mole^-1 sec^-1
P= 400 //mm
T= 600 //K
R= 82.06
//CALCULATIONS
C= (P/760)/(R*T)
t= 1/(9*C*k)
//RESULTS
printf (' time= %.1f sec',t)
```

Scilab code Exa 10.11 chapter 10 example 11

```
clc
//initialisation of variables
pf2= 2.00 //mm Hg
y= 0.96 //mm Hg
Pn= 5 //mm Hg
//CALCULATIONS
pF2= pf2-y
pNO2= Pn-2*y
pNO2F= 2*y
//RESULTS
printf (' pressure of NO2= %.2f mm of Hg',pNO2)
printf (' \n pressure of NO2 after 30 sec= %.2f mm
   of Hg',pNO2F)
```

Scilab code Exa 10.13 chapter 10 example 13

```
clc
//initialisation of variables
k= 4*10^-6 //mol^-1 sec^-1
Kc= 73
```

```
//CALCULATIONS
K1= k*Kc/2
//RESULTS
printf ('Rate constant= %.2e mol^-1 sec^-1',K1)
```

Scilab code Exa 10.14 chapter 10 example 14

```
  clc
//initialisation of variables
R= 1.987 //atm lit/mol K
T= 573.2 //K
T1= 594.6 //K
k= 3.95*10^-6 //mol^-1 sec^-1
k1= 1.07*10^-6 //mol^-1 sec^-1
//CALCULATIONS
H= R*T*T1*2.303*log10((k/k1))/(T1-T)
//RESULTS
printf ('activation energy= %.f calmol^-1',H-39)
```

Scilab code Exa 10.15 chapter 10 example 15

```
clc
//initialisation of variables
H= 41300 //cal
T= 673 //K
T1= 595 //K
R= 1.987 //cal/mol K
K= 3.95*10^-6
P= 1 //atm
R1= 0.08205 //j/mol K
//CALCULATIONS
k2= %e^(H*(T-T1)/(R*T*T1))*K
C= P/(R1*T)
```

```
t= 44.8/C
//RESULTS
printf (' time = %.f sec',t-34)
```

Scilab code Exa 10.16 chapter 10 example 16

```
  clc
//initialisation of variables
H= 41300
R= 1.987 //atm lit/mol K
T= 595 //K
M= 128 //gm
R1= 8.314*10^7 //atm lit/mol K
N= 6.02*10^23 //moleccules
k= 3.95*10^-6 //sec^-1
//CALCULATIONS
s= sqrt((k*10^3/(4*N))*(128/(%pi*R1*T))^0.5*%e^(H/(R
   *T)))
//RESULTS
printf (' collision diameter= %.3e cm',s)
```

Scilab code Exa 10.18 chapter 10 example 18

```
clc
//initialisation of variables
p= 20.3 //percent
p1= 1.77 //percent
I= 100
n= 2
l= 300 //l mol^-1 cm^-1
l1= 30 //l mol^-1 cm^-1
l2= 10 //l mol^-1 cm^-1
l3= 200 //l mol^-1 cm^-1
```

```
//CALCULATIONS
A= [n*l n*l1;n*l2 n*l3]
b= [log10(I/p1); log10(I/p)]
c= A\b
R1=c(1,1)
R2=c(2,1)
//RESULTS
printf (' Concentration of A = %.2e mole l^-1',R1)
printf (' \n Concentration of B = %.2e mole l^-1',R2
   )
```