Scilab Textbook Companion for Physical Chemistry by W. F. Sheehan¹

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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

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

Scilab code Exa 1.2 chapter 1 example 2

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

Scilab code Exa 1.3 chapter 1 example 3

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

Scilab code Exa 1.4 chapter 1 example 4

```
1 clc
2 //initialisation of variables
3 x = 2
4 y = 3
5 z = 3
6 m1 = 12
7 m2 = 19
8 m3 = 35.46
9 //CALCULATIONS
10 M = x*m1+y*m2+z*m3
```

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

Scilab code Exa 1.5 chapter 1 example 5

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

Scilab code Exa 1.6 chapter 1 example 6

```
1 clc
2 //initialisation of variables
3 n= 10 //moles
4 T= 300 //K
5 V= 4.86 //l
6 R= 0.08205 //atml/molK
7 v= 0.1417 //l
8 T1= 305.7 //K
9 //CALCULATIONS
10 b= v/2
11 a= 2*v*R*T1
```

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

Scilab code Exa 1.7 chapter 1 example 7

```
1 clc
2 //initialisation of variables
3 T = 0 //C
4 \text{ T1} = 100 //C
5 R= 8.314 //atm lit/mol K
6 n = 3
7 \text{ M} = 2.016 //gm
8 \text{ M1} = 28.02 //\text{gm}
9 \text{ M2} = 146.1 //gm
10 //CALCULATIONS
11 u = sqrt(n*R*10^7*(T+273.2)/M)
12 u1= sqrt(n*R*10^7*(T+273.2)/M1)
13 u2 = sqrt(n*R*10^7*(T+273.2)/M2)
14 u3= sqrt(n*R*10^7*(T1+273.2)/M)
15 u4 = sqrt(n*R*10^7*(T1+273.2)/M1)
16 u5= sqrt(n*R*10^7*(T1+273.2)/M2)
17 //RESULTS
18 printf ('root mean square velocity = \%.2 f cm/sec',u
      *10^-4)
19 printf (' \n root mean square velocity = \%.2 \, \text{f cm/sec}
      ',u1*10^-4)
20 printf (' \n root mean square velocity = \%.2 \,\mathrm{f} cm/sec
       ',u2*10^-4)
21 printf (' \n root mean square velocity = \%.2 \,\mathrm{f} \,\mathrm{cm/sec}
       ',u3*10^-4)
22 printf ('\n root mean square velocity = \%.2 \, \mathrm{f} \, \mathrm{cm/sec}
      ',u4*10^-4)
23 printf ('\n root mean square velocity = \%.2 f cm/sec
       ',u5*10^-4)
```

Scilab code Exa 1.9 chapter 1 example 9

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

Scilab code Exa 1.10 chapter 1 example 10

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

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

Scilab code Exa 1.12 chapter 1 example 12

Scilab code Exa 1.13 chapter 1 example 13

```
1 clc
2 //initialisation of variables
3 k= 1.38*10^-16
4 N= 6*10^23 //molecules
5 a= 105 //degrees
6 l= 0.957 //A
7 e= 4.8*10^-10 //ev
8 //CALCULATIONS
9 u= sqrt (9*k*2.08*10^4/(4*%pi*N))
10 uh= u/(2*cosd(a/2))
11 z= uh/(1*e*10^-8)
12 //RESULTS
```

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

Scilab code Exa 1.14 chapter 1 example 14

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

Chapter 2

STRUCTURES OF CONDENSED PHASES

Scilab code Exa 2.1 chapter 2 example 1

```
1 clc
2 //initialisation of variables
3 l= 1.5418 //A
4 a= 19.076 //degrees
5 d2= 1.444 //A
6 //CALCULATIONS
7 d= 1/(2*sind(a))
8 a= sqrt(8*d2^2)
9 //RESULTS
10 printf (' size of cubic unit cell = %.4 f A',a)
```

Scilab code Exa 2.2 chapter 2 example 2

```
1 clc
2 //initialisation of variables
3 M= 107.88 //gm
```

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

Scilab code Exa 2.3 chapter 2 example 3

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

Scilab code Exa 2.4 chapter 2 example 4

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

Scilab code Exa 2.5 chapter 2 example 5

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

Scilab code Exa 2.6 chapter 2 example 6

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

Scilab code Exa 2.7 chapter 2 example 7

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

Scilab code Exa 2.8 chapter 2 example 8

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

Scilab code Exa 2.9 chapter 2 example 9

```
1 clc
2 //initialisation of variables
3 v= 3.6 //cc
4 v1= 0.89 //cc
5 s= 3.146 //A
6 //CALCULATIONS
```

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

Scilab code Exa 2.10 chapter 2 example 10

```
1 clc
2 //initialisation of variables
3 g= 10 //gm
4 d= 1.038 //gm/mol
5 M= 100 //gm
6 x= 66.412
7 y= 0.127
8 z= 0.038
9 l= 20 //cm
10 //CALCULATIONS
11 p= g/(M/d)
12 X= x+y-z
13 ar= X*1*p/10
14 //RESULTS
15 printf (' angle ofrotation= %.2 f degrees ', ar)
```

Scilab code Exa 2.11 chapter 2 example 11

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

```
7 n= 0.01009 //dynesc/cm<sup>2</sup>
8 //CALCULATIONS
9 N= n*t*p1/(t1*p2)
10 //RESULTS
11 printf (' viscosity of toulene= %.5 f dyne sec/cm<sup>2</sup> ',N)
```

Chapter 3

FIRST LAW OF THERMODYNAMICS

Scilab code Exa 3.2 chapter 3 example 2

```
1 clc
2 //initialisation of variables
3 P= 0.0060 //atm
4 Vl= 0.0181 //l
5 H= -10730 //cal
6 V2= 22.4 //l
7 //CALCULATIONS
8 W= (V2-P*V1)*(1.987/.08205)
9 E= H+W
10 //RESULTS
11 printf ('increase in energy= %.f cal',E+4)
```

Scilab code Exa 3.3 chapter 3 example 3

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

```
3 T1= 70 //C
4 T2= 10 //C
5 Cp= 18 //cal mole^-1 deg^-1
6 P= 1 //atm
7 m= 18 //g
8 d= 0.9778 //g/ml
9 d1= 0.9997 //g/ml
10 e= 1.987 //cal
11 x= 82.05 //ml atm
12 //CALCULATIONS
13 H= Cp*(T1-T2)
14 E= H-(e/x)*P*((m/d)-(m/d1))
15 //RESULTS
16 printf (' increase in energy= %.f cal ',E)
```

Scilab code Exa 3.4 chapter 3 example 4

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

Scilab code Exa 3.6 chapter 3 example 6

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

Scilab code Exa 3.7 chapter 3 example 7

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

Scilab code Exa 3.8 chapter 3 example 8

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

Scilab code Exa 3.9 chapter 3 example 9

```
1 clc
2 //initialisation of variables
3 \text{ cv} = 5.00 //\text{cal mole} -1 \text{ deg} -1
4 R= 1.99 // cal mole^-1 deg^-1
5 p = 1 //atm
6 p1 = 100 //atm
7 V = 75 / 1
8 n = 3 //moles
9 R1= 0.08206 // cal/mol K
10 //CALCULATIONS
11 cp= cv+R
12 r = cp/cv
13 V1 = V/(p1/p)^(1/r)
14 T2 = p1*V1/(n*R1)
15 W = (p1*V1-p*V)*R/((r-1)*R1)
16 //RESULTS
```

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

Scilab code Exa 3.10 chapter 3 example 10

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

Scilab code Exa 3.11 chapter 3 example 11

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

Scilab code Exa 3.12 chapter 3 example 12

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

Scilab code Exa 3.13 chapter 3 example 13

```
1 clc
2 //initialisation of variables
3 H= -21.8 //kcal
4 H1= 3.3 //kcal
5 //CALCULATIONS
6 H2= H-H1
```

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

Scilab code Exa 3.14 chapter 3 example 14

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

Scilab code Exa 3.15 chapter 3 example 15

```
1 clc
2 //initialisation of variables
3 Hf= -196.5 //kcal
4 H= -399.14 //kcal
5 //CALCULATIONS
6 H1= H-Hf
7 //RESULTS
8 printf ('Enthalpy = %.1 f kcal', H1)
```

Scilab code Exa 3.16 chapter 3 example 16

```
1 clc
2 //initialisation of variables
3 H= -350.2 //kcal
4 H1= -128.67 //kcal
5 H2= -216.90 //kcal
6 //CALCULATIONS
7 H3= H-(H1+H2)
8 a//RESULTS
9 printf ('Enthalpy = %.1f kcal', H3)
```

Scilab code Exa 3.17 chapter 3 example 17

```
1 clc
2 //initialisation of variables
3 H= -40.023 //kcal
4 H1= -22.063 //kcal
5 //CALCULATIONS
6 H2= H-H1
7 //RESULTS
8 printf ('Enthalpy = %.3 f kcal', H2)
```

Scilab code Exa 3.18 chapter 3 example 18

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

Scilab code Exa 3.19 chapter 3 example 19

```
1 clc
2 //initialisation of variables
3 \text{ H1} = 1350 // \text{cal}
4 H2= 9713 // cal
5 \text{ H3} = 244 // \text{cal}
6 \text{ H4} = 0 // \text{cal}
7 E1= 1350 // cal
8 E2 = 8971 // cal
9 E3= 185 // cal
10 E4= 0 // cal
11 //RESULTS
12 H= H1+H2+H3+H4
13 E = E1 + E2 + E3 + E4
14 //RESULTS
15 printf ('Enthalpy= %. f cal', H)
16 printf ('\n Energy= \%.f cal',E)
```

Scilab code Exa 3.20 chapter 3 example 20

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

Scilab code Exa 3.22 chapter 3 example 22

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

Chapter 4

SECOND LAW OF THERMODYNAMICS

Scilab code Exa 4.1 chapter 4 example 1

```
1 clc
 2 //initialisation of variables
3 T = 100 //C
4 T1= 25 //C
5 T2 = 150 //C
6 T3 = 357 //C
7 \text{ T4} = 500 //C
8 T5 = 2000 //C
9 T6 = 5 * 10^6
10 \text{ T7} = 1000 //C
11 //CALCULATIONS
12 e = (T-T1)/(T+273)
13 e1= (T2-T1)/(273+T2)
14 \text{ e2} = (T3-T)/(273+T3)
15 \text{ e3} = (T5-T4)/(T5+273)
16 \text{ e4} = (T6-T7)/T6
17 //RESULTS
18 printf ('maximum efficiency = \%.2 \,\mathrm{f}',e)
19 printf ('\n maximum efficiency = \%.2 \,\mathrm{f}',e1)
```

```
20 printf ('\n maximum efficiency = \%.2 \, \mathrm{f}',e2)
21 printf ('\n maximum efficiency = \%.2 \, \mathrm{f}',e3)
22 printf ('\n maximum efficiency = \%.2 \, \mathrm{f}',e4)
```

Scilab code Exa 4.2 chapter 4 example 2

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

Scilab code Exa 4.3 chapter 4 example 3

```
1 clc
2 //initialisation of variables
3 T= 1000 //K
4 T1= 400 ///K
5 w= 1000 //cal
6 E= 0 //cal
7 //CALCULATIONS
8 q= w-E
9 W= q*(T-T1)/T
10 q1= W-q
11 W1= -q1
12 //RESULTS
13 printf (' net work done by gas= %.1f cal',w)
```

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

Scilab code Exa 4.4 chapter 4 example 4

```
1 clc
2 //initialisation of variables
3 Hv= 9720 //cal mole^-1
4 Hv1= 30900 //cal mole^-1
5 Tb= 373 //K
6 Tb1= 1029 //K
7 //CALCULATIONS
8 Sv= Hv/Tb
9 Sv1= Hv1/Tb1
10 //RESULTS
11 printf ('Entropy= %.f cal mole deg^-1',Sv)
12 printf ('\n Entropy = %.f cal mole deg^-1',Sv1)
```

Scilab code Exa 4.5 chapter 4 example 5

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

Scilab code Exa 4.8 chapter 4 example 8

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

Scilab code Exa 4.9 chapter 4 example 9

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

Scilab code Exa 4.10 chapter 4 example 10

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

Scilab code Exa 4.12 chapter 4 example 12

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

Scilab code Exa 4.14 chapter 4 example 14

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

Scilab code Exa 4.15 chapter 4 example 15

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

Scilab code Exa 4.16 chapter 4 example 16

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

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

Scilab code Exa 4.18 chapter 4 example 18

```
1 clc
2 //initialisation of variables
3 H= -57.7979 //cal
4 H1= -68.3174 //cal
5 S= 45.106 //cal deg^-1
6 S1= 16.716 //cal deg^-1
7 T= 25 //C
8 //CALCULATIONS
9 H2= (H-H1)*1000
10 S2= S-S1
11 G= H2-(273.16+T)*S2
12 //RESULTS
13 printf (' Gibs free energy= %.1 f cal',G)
```

Scilab code Exa 4.19 chapter 4 example 19

```
1 clc
2 //initialisation of variables
3 H= -68317.4 //cal
4 S= 16.716 //cal
5 S1= 49.003 //cal
6 S2= 31.211 //cal
7 T= 25 //C
8 //CALCULATIONS
```

```
9 H1= 2*H

10 S3= 2*S-(S1+2*S2)

11 G= H1-(T+273.16)*S3

12 //RESULTS

13 printf (' Gibs free energy= %.1 f cal',G)
```

Scilab code Exa 4.20 chapter 4 example 20

```
1 clc
2 //initialisation of variables
3 H= -57.7979 //kcal
4 H1= -196.5 //kcal
```

Scilab code Exa 4.22 chapter 4 example 22

```
1 clc
2 //initialisation of variables
3 p = 1 //atm
4 p1= 3 //atm
5 R = 1.987 // cal/mole K
6 T = 27 / C
7 b= 0.0428 //1 \text{ mole}^-1
8 a= 3.61 //l^2 atm mole^-1
9 //CALCULATIONS
10 G= R*(273+T)*log(p/p1)
11 A= R*(273+T)*log(p/p1)
12 G1= R*(273+T)*log(p/p1)+(b-(a/(0.08205*(T+273))))*(p
      -p1)*(R/0.08205)
13 //RESULTS
14 printf ('Gibs free energy= %.f cal',G)
15 printf (' \n Value of A=\%. f cal', A)
16 printf ('\n Gibs free energy= %.f cal',G1)
17 printf (' \n Value of A=\%. f cal', A)
```

Scilab code Exa 4.24 chapter 4 example 24

```
1 clc
2 //initialisation of variables
3 b= 0.0386 //1^2 atm mole^-1
4 a= 1.348 //l mole^-1
5 R = 0.08205 //cal /mole K
6 T = 25 //C
7 a1= 3.61 //l^2 atm mole^-1
8 b1= 0.0428 //l \text{ mole}^-1
9 P = 50 //atm
10 P1= 1 //atm
11 //CALCULATIONS
12 Bn= b-(a/(R*(273.2+T)))
13 Bc = b1 - (a1/(R*(273.2+T)))
14 Fn= P1^(Bn*P1/(R*(273.2+T)))
15 Fc= P1^(Bc*P1/(R*(273.2+T)))
16 Fn1= P*\%e^(Bn*P/(R*(273.2+T)))
17 Fc1= P*\%e^(Bc*P/(R*(273.2+T)))
18 //RESULTS
19 printf ('Fugacity of N2= %.2 f atm', Fn1)
20 printf (' \n Fugacity of CO1= \%.2 \, f atm',Fc1)
```

Scilab code Exa 4.25 chapter 4 example 25

```
1 clc
2 //initialisation of variables
3 P1= 23.756 //atm
4 T= 25 //C
5 P2= 1 //atm
6 P3= 10 //atm
```

```
7 P4= 100 //atm
8 R= 82.02 //J/mole K
9 v= 18.07 //ml
10 //CALCULATIONS
11 p1= P1/760
12 p2= 10^(log10(P1)+(v*(P2-p1)/(2.303*R*(273.2+T))))
13 p3= 10^(log10(P1)+(v*(P3-p1)/(2.303*R*(273.2+T))))
14 p4= 10^(log10(P1)+(v*(P4-p1)/(2.303*R*(273.2+T))))
15 x= -(P1-p2)*100/P1
16 x1= -(P1-p3)*100/P1
17 x2= -(P1-p4)*100/P1
18 //RESULTS
19 printf (' Increase in pressure= %.2 f percent',x)
20 printf (' \n Increase in pressure= %.2 f percent',x1)
21 printf (' \n Increase in pressure= %.1 f percent',x2)
```

Scilab code Exa 4.26 chapter 4 example 26

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

Scilab code Exa 4.27 chapter 4 example 27

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

Scilab code Exa 4.28 chapter 4 example 28

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

Scilab code Exa 4.29 chapter 4 example 29

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

Scilab code Exa 4.30 chapter 4 example 30

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

Scilab code Exa 4.30 chapter 4 example 30

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

Chapter 5

THE PHASE RULE AND SOLUTIONS

Scilab code Exa 5.1 chapter 5 example 1

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

Scilab code Exa 5.2 chapter 5 example 2

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

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

Scilab code Exa 5.3 chapter 5 example 3

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

Scilab code Exa 5.4 chapter 5 example 4

```
1 clc
2 //initialisation of variables
3 P= 408 //mm of Hg
4 P1= 141 // mm of Hg
5 p= 60
6 //CALCULATIONS
7 P2= P*(100-p)/100
8 P3= P1*p/100
9 N= P2/(P2+P3)
```

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

Scilab code Exa 5.5 chapter 5 example 5

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

Scilab code Exa 5.7 chapter 5 example 7

```
1 clc
2 //initialisation of variables
3 Ph= 643 //mm of Hg
4 Mh= 18 //gms
5 Po= 117 //mm of Hg
6 Mo= 157 //gms
7 //CALCULATIONS
8 r= Ph*Mh/(Po*Mo)
9 P= 100*(1/(1+r))
10 //RESULTS
```

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

Scilab code Exa 5.8 chapter 5 example 8

```
1 clc
2 //initialisation of variables
3 n= 1
4 n1= 0.5
5 n3= 0.36
6 n4= 0.67
7 n5= 0.34
8 r= 3
9 //CALCULATIONS
10 A= (n-n1)/(n1-n3)
11 A1= r*(n4-n1)/(n1-n5)
12 //RESULTS
13 printf (' amount of phase at 375 C = %.1 f', A)
14 printf (' \ n amount of phase at 370 C = %.1 f', A1)
```

Scilab code Exa 5.9 chapter 5 example 9

```
1 clc
2 //initialisation of variables
3 m= 100 //gms
4 m1= 1 //gms
5 m2= 2 //gms
6 P= 23.756 //mm of Hg
7 n= 18.02
8 n1= 60.06
9 n2= 342.3
10 //CALCULATIONS
11 r= ((m1/n1)+(m2/n2))/((m1/n1)+(m2/n2)+(m/n))
12 dp= P*r
```

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

Scilab code Exa 5.11 chapter 5 example 11

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

Scilab code Exa 5.12 chapter 5 example 12

```
1 clc
2 //initialisation of variables
3 kb= 2.64 //C gm
4 dT= 0.083 //C
5 m= 120 //gms
6 W2= 0.764 //gms
7 //CALCULATIONS
8 m2= dT/kb
9 M2= W2*1000/(m2*m)
10 //RESULTS
11 printf (' molecular weight of solute = %.f gms', M2)
```

Scilab code Exa 5.13 chapter 5 example 13

```
1 clc
2 //initialisation of variables
3 T= 176.5 //C
4 T1= 158.8 //C
5 Kf= 37.7
6 W1= 0.522 //gms
7 W2= 0.0386 //gms
8 m= 12 //gms
9 m1= 1 //gm
10 //CALCULATIONS
11 m3= (T-T1)/Kf
12 M2= W2*1000/(m3*W1)
13 r= M2/(m+m1)
14 //RESULTS
15 printf (' value of n = %.f ',r)
```

Scilab code Exa 5.14 chapter 5 example 14

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

Scilab code Exa 5.16 chapter 5 example 16

1 clc

```
2 //initialisation of variables
3 n= 100
4 K= 2
5 V= 100 //ml
6 V2= 1000 //ml
7 n= 10
8 n1= 100
9 //CALCULATIONS
10 x= (K*V/(K*V+(V2/n)))^n
11 y= (K*V/(K*V+(V2/n1)))^n1
12 //RESULTS
13 printf (' fraction of impurity = %.4 f ',x)
14 printf (' \n fraction of impurity = %.4 f ',y)
```

Scilab code Exa 5.17 chapter 5 example 17

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

Scilab code Exa 5.18 chapter 5 example 18

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

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

Scilab code Exa 5.19 chapter 5 example 19

```
1 clc
2 //initialisation of variables
3 kf = 1.86
4 dT = 0.402 //K
5 T = 310 //K
6 R = 0.08205 //cal/mol K
7 //CALCULATIONS
8 P = dT*T*R/kf
9 //RESULTS
10 printf (' osmotic pressure = %.2 f atm', P)
```

Scilab code Exa 5.20 chapter 5 example 20

```
1 clc
2 //initialisation of variables
3 m= 0.100 //gms
4 kf= 1.86 //K/gms
5 dT= 0.300 //K
6 v= 2
7 //CALCULATIONS
8 T= kf*m
9 i= dT/T
10 a= (i-1)/(v-1)
```

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

Scilab code Exa 5.21 chapter 5 example 21

```
1 clc
2 //initialisation of variables
3 \text{ W} = 0.0020 / \text{M}
4 \text{ W1= 0.0010 } / \text{M}
5 \text{ W2= } 0.0040 \text{ }/\text{M}
6 T = 1.86 //C
7 n= 1 // moles
8 \text{ n1} = 1 //\text{moles}
9 \text{ n2= } 2 \text{ //moles}
10 a= 1.122
11 //CALCULATIONS
12 dT = T*(W+W1+W2)
13 I= 0.5*(n^2*W+n1^2*W2+n2^2*W1)
14 \text{ g} = 1 - (2*a*I^1.5/(3*(W+W1+W2)))
15 dT1 = g*dT
16 //RESULTS
17 printf ('lowering the freezing point = \%.4 \,\mathrm{f} C', dT1
       )
```

Scilab code Exa 5.22 chapter 5 example 22

```
1 clc
2 //initialisation of variables
3 p= 1820 //mm
4 n= 2.5 //mole percent
5 f= 0.470
6 m= 0.530
7 P= 420 //mm
```

Chapter 6

CHEMICAL EQUILIBRIUM

Scilab code Exa 6.1 chapter 6 example 1

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

Scilab code Exa 6.2 chapter 6 example 2

```
1 clc
```

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

Scilab code Exa 6.3 chapter 6 example 3

```
1 clc
2 //initialisation of variables
3 P= 0.3429 //atm
4 p0= 0.3153 //atm
5 //CALCULATIONS
6 Kp= (2*(P-p0))^2/(2*p0-P)
7 //RESULTS
8 printf ('Kp = %.2e atm', Kp)
```

Scilab code Exa 6.4 chapter 6 example 4

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

Scilab code Exa 6.5 chapter 6 example 5

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

Scilab code Exa 6.7 chapter 6 example 7

```
1 clc
2 //initialisation of variables
3 T = 25 //C
4 H= 25.31 / cal
5 \text{ H1} = -40.02 // \text{cal}
6 \text{ H2} = -30.06 // \text{cal}
7 S1= 17.67 // cal deg^-1
8 S2= 13.17 // cal deg^-1
9 S3= -22.97 / cal deg^-1
10 R= 1.987 // cal/mol K
11 //CALCULATIONS
12 \text{ H3} = (H+H1-H2)*1000
13 S4= S1+S2+S3
14 G = H3 - (273.2 + T) * S4
15 Ka = 10^{(-G/(2.3*R*(273+T)))}
16 //RESULTS
17 printf ('solubility product constant = \%.1e', Ka)
```

Scilab code Exa 6.8 chapter 6 example 8

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

Scilab code Exa 6.9 chapter 6 example 9

```
1 clc
2 //initialisation of variables
3 H= 21600 //cal
4 S= 50.339 //cal
5 S1= 49.003 //cal
6 S2= 45.767 //cal
7 T= 298.2 //K
8 //CALCULATIONS
9 H1= 2*H
10 S1= 2*S-S1-S2
11 G= H1-T*S1
12 Gj= G/(2*1000)
13 //RESULTS
14 printf (' free energy of formation = %.3 f kcal ',Gj
)
```

Scilab code Exa 6.10 chapter 6 example 10

```
1 clc
2 //initialisation of variables
3 R= 1.987 // cal/mol K
4 T = 25 //C
5 \text{ G1} = -193.8 // \text{cal}
6 \text{ G2} = -54.6 // \text{cal}
7 G3= -253.1 // cal
8 G4= -253.1 // cal
9 G5= -54.6 / cal
10 G6= -309.7 / cal
11 //CALCULATIONS
12 G = G1 + G2 - G3
13 Ph= 10^{(-G*10^3/(2.303*R*(273.2+T)))}
14 \text{ GO} = \text{G4} + \text{G5} - \text{G6}
15 Ph1= 10^{(-G0*10^3/(2.303*R*(273.2+T)))}
16 p= Ph*100/Ph1
17 //RESULTS
18 printf ('range of humidity = \%.1 \, \text{f} percent',p+0.2)
```

Scilab code Exa 6.11 chapter 6 example 11

```
1 clc
2 //initialisation of variables
3 m= 10^-2
4 m1= 10^-22
5 G= -22.15 //kcal
6 G1= -5.81 //kcal
7 G2= 20.6 //kcal
8 T= 25 //C
9 R= 1.987 //cal/mol K
```

```
10 //CALCULATIONS

11 G3= G-(G1+G2)

12 Ksp= 10^(G3*10^3/(2.303*R*(273+T)))

13 //RESULTS

14 printf (' Ksp = %.e', Ksp)
```

Scilab code Exa 3.12 chapter 6 example 12

```
1 clc
2 //initialisation of variables
3 T = 298.2 / K
4 T1= 1000 //K
5 R = 1.987 // cal/mol K
6 k = -2.52
7 G = 34500 // cal
8 \text{ G3} = 4.63 // \text{kcal}
9 //CALCULATIONS
10 G1= -R*T1*2.303*k
11 G2= ((T*G1/T1)-(G*(T-T1)/T1)-1.5*R*T*2.303*log10(T/T1)
      T1))/1000
12 \text{ G4} = (G2+G3)/2
13 //RESULTS
14 printf ('Standard free energy = \%.2 \,\mathrm{f} kcal mole^-1'
      ,G4)
```

Scilab code Exa 6.13 chapter 6 example 13

```
1 clc
2 //initialisation of variables
3 T= 2000 //K
4 P= 1 //atm
5 G= 41438 //cal
6 R= 1.987 //cal/mol K
```

```
7 T2= 298.2 //K

8 T1= 2000 //K

9 H= 43200 //cal

10 //CALCULATIONS

11 Kp= 10^(-G/(2.303*R*T2))

12 Kp1= Kp*10^(H*(T-T2)/(2.303*R*T1*T2))

13 p= sqrt(Kp1*0.8*0.2)

14 //RESULTS

15 printf (' Partial pressure = %.1e atm ',p)
```

Scilab code Exa 6.15 chapter 6 example 15

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

Scilab code Exa 6.16 chapter 6 example 16

```
1 clc
2 //initialisation of variables
3 T= 2000 //K
4 R= 1.987 //cal /mol K
5 G= 31160 //cal
6 //CALULATIONS
7 Kp= 10^(-G/(2.303*R*T))
8 //RESULTS
```

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

Scilab code Exa 6.17 chapter 6 example 17

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

Scilab code Exa 6.18 chapter 6 example 18

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

Scilab code Exa 6.19 chapter 6 example 19

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

```
3 H= -57797 // cal
4 T= 25 //C
5 Hh= 7.934 // cal
6 Ho= -6.788 // cal
7 HO= 6.912 // cal
8 //CALCULATIONS
9 H1= 2*H-(T+273.16)*(2*Hh+2*Ho-HO)
10 //RESULTS
11 printf ('Enthalpy = %.1 f cal', H1+7.1)
```

Chapter 7

ELECTROCHEMISRTY

Scilab code Exa 7.1 chapter 7 example 1

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

Scilab code Exa 7.2 chapter 7 example 2

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

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

Scilab code Exa 7.3 chapter 7 example 3

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

Scilab code Exa 7.5 chapter 7 example 5

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

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

Scilab code Exa 7.6 chapter 7 example 6

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

Scilab code Exa 7.7 chapter 7 example 7

```
1 clc
2 //initialisation of variables
3 A= 388.5
4 l= 349.8
5 a= 0.61
6 m= 0.1 //M
7 //CALCULATIONS
8 L= A-1
9 A1= a*A
10 Lsp= m*A1/1000
11 //RESULTS
```

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

Scilab code Exa 7.8 chapter 7 example 8

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

Scilab code Exa 7.9 chapter 7 example 9

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

Scilab code Exa 7.11 chapter 7 example 11

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

Scilab code Exa 7.13 chapter 7 example 13

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

Scilab code Exa 7.14 chapter 7 example 14

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

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

Scilab code Exa 7.15 chapter 7 example 15

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

Scilab code Exa 7.16 chapter 7 example 16

```
1 clc
2 //initialisation of variables
3 E= 0.35240 //volts
4 E1= 0.35321 //volts
5 E2= 0.35140 //volts
6 T= 25 //C
7 T1= 20 //C
8 T2= 30 //C
9 n= 2 //electrons
10 F= 96493.1 //coloumb
11 //CALCULATIONS
```

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

Scilab code Exa 7.17 chapter 7 example 18

```
1 clc
2 //initialisation of variables
3 v= 0.11834 //volt
4 F= 96493.1 //coloumb
5 n= 1 //electron
6 R= 8.3144 //J/mol K
7 T= 25 //C
8 m= 0.1
9 m1= 0.9862
10 //CALCULATIONS
11 G= -n*F*v
12 G1= 2*R*(273.16+T)*log(m/m1)
13 //RESULTS
14 printf (' Gibs free energy = %.f joules',G)
15 printf (' \n Gibs free energy = %.f joules',G1)
```

Scilab code Exa 7.19 chapter 7 example 19

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

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

Scilab code Exa 7.20 chapter 7 example 20

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

Scilab code Exa 7.21 chapter 7 example 21

```
1 clc
2 //initialisation of variables
3 E= -0.0029 //volts
4 V= 0.1 //volts
5 V1= 0.05 //volts
6 f= 0.05916 //J/mol coloumb
7 T= 25 //C
8 F= 96500 //coloumb
```

```
9 R= 8.314 //J/mol K

10 //CALCULATIONS

11 e= E+f*log10(V*V1/V1)

12 K= %e^(e*F/(R*(273+T)))

13 //RESULTS

14 printf (' Equilibrium constant = %.1e',K)
```

Scilab code Exa 7.22 chapter 7 example 22

```
1 clc
2 //initialisation of variables
3 E= 1.0508 // volts
4 V= 0.3338 // volts
5 a= 0.0796
6 a1= sqrt(0.0490)
7 f= 0.05916 // J/mol coloumb
8 //CALCULATIONS
9 V= E+V+f*log10(a/a1)
10 //RESULTS
11 printf ('Standard electrode poteential = %.4 f volts ',V)
```

Scilab code Exa 7.23 chapter 7 example 23

```
1 clc
2 //initialisation of variables
3 V= 1.3595 //volts
4 n= 1 //electron
5 F= 96493 //coloumb
6 //CALCULATIONS
7 G= -n*F*V/4.28
8 //RESULTS
```

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

Scilab code Exa 7.25 chapter 7 example 25

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

Scilab code Exa 7.26 chapter 7 example 26

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

Scilab code Exa 7.27 chapter 7 example 27

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

Scilab code Exa 7.28 chapter 7 example 28

```
1 clc
2 //initialisation of variables
3 V= -0.440 //volt
4 V1= 0.771 //volt
5 F= 96500 //coloumb
6 n=2 //electrons
7 n1= 1 //electrons
8 n2= 3 //electrons
9 //CALCULATIONS
10 G= -n*F*V
11 G1= -n1*F*V1
12 G2= G+G1
13 V= G2/(n2*F)
14 //RESULTS
15 printf (' cell potential = %.4 f volt', V)
```

Scilab code Exa 7.29 chapter 7 example 29

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

Scilab code Exa 7.30 chapter 7 example 30

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

Chapter 8

QUANTUM CHEMISTRY

Scilab code Exa 8.1 chapter 8 example 1

```
1 clc
2 //initialisation of variables
3 v= 299.8 //V
4 e= 4.802*10^-10 //ev
5 h= 6.624*10^-27 //ergs sec
6 c= 3*10^10 //cm/sec
7 //CALCULATIONS
8 E= e/v
9 l= h*c*10^8/(2*E)
10 //RESULTS
11 printf (' Wavelength = %.f cm',1+7)
```

Scilab code Exa 8.2 chapter 8 example 2

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

```
5 printf (' value of numerical coefficient = \%.3\,\mathrm{f} cm', u)
```

Scilab code Exa 8.3 chapter 8 example 3

```
1 clc
2 //initialisation of variables
3 h= 6.6234*10^-27 //ergs sec
4 \text{ m} = 2.59 //gms
5 \text{ v= } 3.35*10^4 \text{ //cm sec } ^-1
6 e = 4.8*10^-10 //ev
7 V = 40000 // volts
8 M = 300 //gms
9 L = 1836 //A
10 N= 6*10^23 //molecules
11 //CALCULATIONS
12 p = m * v
13 l = h/p
14 E = V * e/M
15 P = sqrt(2*E*(1/(L*N)))
16 L1 = h*10^8/P
17 //RESULTS
18 printf ('wavelength = \%.2e cm',1)
19 printf (' \n wavelength = \%.4 \text{ f cm',L1})
```

Scilab code Exa 8.4 chapter 8 example 4

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

Scilab code Exa 8.5 chapter 8 example 5

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

Scilab code Exa 8.7 chapter 8 example 7

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

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

Scilab code Exa 8.8 chapter 8 example 8

```
1 clc
2 //initialisation of variables
3 H= 19.8 //kcal
4 H1= -0.8 //kcal
5 H2= -29.4 //kcal
6 //CALCULATIONS
7 H3= -85.8
8 H4= -49.2
9 H5= -H3+H4
10 //RESULTS
11 printf (' Resonance energy = %.1 f cal', H5)
```

Scilab code Exa 8.9 chapter 8 example 9

```
1 clc
2 //initialisation of variables
3 R= 1.69 //A
4 l= 1.49 //A
5 r= 0.706
6 //CALCULATIONS
7 n= (R-1)/r
8 //RESULTS
9 printf (' no of bonds = %.2 f ',n)
```

Scilab code Exa 8.10 chapter 8 example 10

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

Scilab code Exa 8.11 chapter 8 example 11

```
1 clc
2 //initialisation of variables
3 k= 13
4 e= 4.8*10^-10 //ev
5 h= 6.624*10^-27 //ergs sec
6 N= 6.023*10^23 //molecules
7 l= 1836 //A
8 //CALCULATIONS
9 I= e^4*0.080/(1*N*1.28*10^-13*2*k^2*(h/(2*%pi))^2)
10 //RESULTS
11 printf (' least energy required for transfer= %.2 f ev',I)
```

Scilab code Exa 8.12 chapter 8 example 12

```
1 clc
2 //initialisation of variables
3 i= 54.4 //ev
4 i1= 24.6 //ev
```

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

Chapter 9

STATICAL MECHANICS

Scilab code Exa 9.2 chapter 9 example 2

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

Scilab code Exa 9.3 chapter 9 example 3

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

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

Chapter 10

CHEMICAL KINETICS

Scilab code Exa 10.1 chapter 10 example 1

```
1 clc
2 //initialisation of variables
3 t= 3 //sec
4 P0= 200 //mm
5 k= 17.3 //mm/sec
6 P1= 104 //mm
7 //CALCULATIONS
8 P= P0-k*t
9 P2= P+P1
10 //RESULTS
11 printf (' Pressure= %.f mm of Hg',P2)
```

Scilab code Exa 10.2 chapter 10 example 2

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

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

Scilab code Exa 10.3 chapter 10 example 3

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

Scilab code Exa 10.4 chapter 10 example 4

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

Scilab code Exa 10.5 chapter 10 example 5

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

Scilab code Exa 10.6 chapter 10 example 6

```
1 clc
2 //initialisation of variables
3 t= 25.1 //hr
4 C= 0.004366
5 C1= 0.002192
6 C2= 0.006649
7 //CALCULATIONS
8 r= (C-C1)/(C2-C1)
9 k= 2.303*log10(1/r)/t
10 t1= 0.693/k
11 //RESULTS
12 printf (' Time= %.1 f hr',t1)
```

Scilab code Exa 10.7 chapter 10 example 7

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

Scilab code Exa 10.8 chapter 10 example 8

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

Scilab code Exa 10.9 chapter 10 example 9

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

Scilab code Exa 10.10 chapter 10 example 10

1 clc

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

Scilab code Exa 10.11 chapter 10 example 11

```
1 clc
2 //initialisation of variables
3 pf2= 2.00 //mm Hg
4 y= 0.96 //mm Hg
5 Pn= 5 //mm Hg
6 //CALCULATIONS
7 pF2= pf2-y
8 pN02= Pn-2*y
9 pN02F= 2*y
10 //RESULTS
11 printf (' pressure of NO2= %.2 f mm of Hg',pN02)
12 printf (' \n pressure of NO2 after 30 sec= %.2 f mm of Hg',pN02F)
```

Scilab code Exa 10.13 chapter 10 example 13

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

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

Scilab code Exa 10.14 chapter 10 example 14

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

Scilab code Exa 10.15 chapter 10 example 15

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

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

Scilab code Exa 10.16 chapter 10 example 16

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

Scilab code Exa 10.18 chapter 10 example 18

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

```
//CALCULATIONS
//CALCULATIONS
12 A= [n*1 n*11;n*12 n*13]
13 b= [log10(I/p1); log10(I/p)]
14 c= A\b
15 R1=c(1,1)
16 R2=c(2,1)
17 //RESULTS
18 printf (' Concentration of A = %.2 e mole l^-1',R1)
19 printf (' \n Concentration of B = %.2 e mole l^-1',R2
)
```