Scilab Textbook Companion for
Physical Chemistry
by G. H. Duffey[1]

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Book Description

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

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

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

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

Contents

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List of Scilab Codes

Chapter 1

Matter and its atomic nature

Scilab code Exa 1.1 Example 1

```
1 clc
2 // Initialization of variables
3 l=0.71 *10^-8 //cm
4 n=200 // lines/cm
5 v=0.00145 // radian
6 // calculations
7 d=1/n
8 phi2=2*l/d +v^2
9 phi=sqrt(phi2)
10 // results
11 printf('Angle required = %.2e radian ',phi)
```

Scilab code Exa 1.2 Example 2

```
1 clc
2 // Initialization of variables
3 angle=37.25 // degrees
4 l=1.539 //A
```

```
5  n=1  //order
6  //calculations
7  d=n*l/(2*sind(angle))
8  //results
9  printf("Interplanar distance = %.3f A",d)
```

Scilab code Exa 1.5 Example 5

```
1  clc
2  //Initialization of variables
3  r1=sqrt(3)
4  r2=1
5  //calculations
6  ratio=r1-r2
7  //results
8  printf('Ratio of radii = %.3f',ratio)
```

Scilab code Exa 1.6 Example 6

```
1   clc
2   //Initialization of variables
3   d=2.64  //g/cc
4   l=4.016*10^-8  //cm
5   n=4
6   M=25.94  //g/mol
7   //calculations
8   m=d*l^3 /n
9   N0=M/m
10  //results
11  printf("Avagadro number = %.3e molecule/mol",N0)
```

Scilab code Exa 1.10 Example 10

```scilab
1  clc
2  // Initialization of variables
3  A=[-1 -1 -1 ]
4  B=[1 1 -1]
5  // calculations
6  Ad=sqrt(1+1+1)
7  Bd=sqrt(1+1+1)
8  dot=A.*B /(Ad*Bd)
9  theta=acosd(dot)
10 // results
11 printf("Angle = %.2f degrees",theta(1,1))
```

Chapter 2

Particles Atomic and subatomic

Scilab code Exa 2.2 Example 2

```
1 clc
2 // Initialization of variables
3 m1=1.008142
4 m2=1.008982
5 // calculations
6 dm=m1-m2
7 dt=abs(dm) *931
8 // results
9 printf("Increase in kinetic energy = %.3 f Mev",dt)
```

Scilab code Exa 2.3 Example 3

```
1 clc
2 // Initialization of variables
3 d=8.642 // g/cc
4 M=112.41 // g/mol
5 ratio=0.01/100
6 nb=2400
```

```
7  //calculations
8  n=d*6.02*10^23 /M
9  sigma=nb*10^-24
10 x=-2.303*log10(ratio) /(sigma*n)
11 //results
12 printf("Thickness = %.3f cm",x)
```

Scilab code Exa 2.4 Example 4

```
1  clc
2  //Initialization of variables
3  M1=4
4  M2=14
5  E=-1.2  //Mev
6  //calculations
7  R1=1.5*10^-13 *(M1)^(1/3)
8  R2=1.5*10^-13 *(M2)^(1/3)
9  V1=2*7*(4.8*10^-10)^2 /(R1+R2)
10 V2=V1/(1.6*10^-6)
11 x=(M1+M2)*V2/M2
12 //results
13 printf("Threshold = %.1f Mev",x)
```

Scilab code Exa 2.6 Example 6

```
1  clc
2  //Initialization of variables
3  t=1622  //years
4  per=1  //percent
5  //calculations
6  Nratio=1-per/100
7  x=t*log10(Nratio) / log10(0.5)
8  //results
```

12

```
9  printf("Time taken = %.1f years",x)
```

Chapter 3

Waves and Quanta

Scilab code Exa 3.9 Example 9

```
1 clc
2 // initialization of variables
3 atoms =5
4 // calculations
5 f =3* atoms
6 fvib = f -3 -3
7 // results
8 printf (" Vibrational degrees of freedom = %d", fvib )
```

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Chapter 4

Molecular energy levels

Scilab code Exa 4.1 Example 1

```
1 clc
2 //initialization of variables
3 B=10.34 //cm^-1
4 c=2.998*10^10 //cm/s
5 h=6.625*10^-27 //erg sec
6 //calculations
7 I=h/(8*%pi^2 *B*c)
8 //results
9 printf("Moment of inertia = %.2e g cm^2",I)
```

Scilab code Exa 4.2 Example 2

```
1 clc
2 //Initialization of variables
3 ma=1.0080
4 mb=35.457
5 Na=6.0232*10^23
6 I=2.707*10^-40 //g cm^2
```

```
7  //calculations
8  mu1=ma*mb/(ma+mb)
9  mu2=mu1/Na
10 r=sqrt(I/mu2)
11 //results
12 printf("Bond length = %.2e cm",r)
```

Scilab code Exa 4.3 Example 3

```
1  clc
2  //Initialization of variables
3  c=2.998*10^10 //cm/s
4  wave=2990 //cm^-1
5  mu=1.627*10^-24 //g
6  //calculations
7  k=mu*(2*%pi*c*wave)^2
8  //results
9  printf("Force constant = %.2e dynes/cm",k)
```

Scilab code Exa 4.4 Example 4

```
1  clc
2  //initialization of variables
3  l1=2886 //cm^-1
4  l2=5668 //cm^-1
5  //calculations
6  wave=2*l1-l2
7  wave2= wave+l1
8  x=wave/(2*wave2)
9  //results
10 printf("anharmonicity constant = %.4f ",x)
```

Chapter 6

Valence electrons in molecules

Scilab code Exa 6.1 Example 1

```
1 clc
2 // initialization of variables
3 a2 =1/8
4 // calculations
5 b2 =1 - a2
6 a1 = sqrt ( a2 )
7 b1 = sqrt ( b2 )
8 // results
9 printf (" Wave function is %.2 f phi1 +%.2 f phi2 " ,a1 ,
    b1 )
```

Scilab code Exa 6.3 Example 3

```
1 clc
2 // initialization of variables
3 sinu =2/ sqrt (3)
4 cosu = sqrt (2/3)
5 // calculations
```

```
6  tanu=sinu/cosu
7  u=atand(sinu/cosu)
8  //results
9  printf("Bond anagle = %.2f degrees",2*u)
```

Scilab code Exa 6.4 Example 4

```
1  clc
2  //initialization of variables
3  cosu=1/sqrt(3)
4  sinu=sqrt(2/3)
5  //calculations
6  f=1/2 + sqrt(3) /2 *cosu + sqrt(3/2) *sinu
7  //results
8  printf("Pauling strength = %d ",f)
```

Scilab code Exa 6.5 Example 5

```
1  clc
2  //initialization of variables
3  alpha=60
4  //calculations
5  cosa=cosd(alpha)
6  sina=sind(alpha)
7  //results
8  printf("Wave function  = %.2f s + %.2f pz",cosa,sina
      )
```

Scilab code Exa 6.9 Example 9

```
1 clc
2 //initialization of variables
3 DHH=103 //kcal/mol
4 //calculations
5 DHHp=0.5*(DHH)
6 //results
7 printf("Bond energy = %.1f kcal/mol",DHHp)
```

Scilab code Exa 6.10 Example 10

```
1 clc
2 //initialization of variables
3 DHH=42 //kcal/mol
4 //calculations
5 DHHp=0.5*(DHH)
6 //results
7 printf("Exchange energy = %.1f kcal/mol",DHHp)
```

Chapter 7

Gases and Introductory stastical thermodynamics

Scilab code Exa 7.2 Example 2

```
1  clc
2  //Initialization of variables
3  h=76  //cm
4  d=13.5951  //g/cc
5  g=980.655  //cm/s^2
6  T=273.15  //K
7  v=22414.6  //cm^3 /mol
8  //calculations
9  P=h*d*g
10 R=P*v/(T)
11 //results
12 printf("Gas constant = %.3e ergs/deg. mol",R)
```

Scilab code Exa 7.3 Example 3

```
1  clc
```

```
2  // Initialization  of  variables
3  cal =4.184*10^7  // ergs
4  R=8.315*10^7  // ergs / deg / mol
5  // calculations
6  Rdash=R/cal
7  // results
8  printf (”R in  calories  = %.3 f  cal /  deg  mol”, Rdash )
```

Scilab code Exa 7.4 Example 4

```
1  clc
2  // Initialization  of  variables
3  R=8.315*10^7  // ergs / deg / mol
4  T=273.2  // deg
5  M=4  //g/mol
6  // calculations
7  u2 =3*T*R/M
8  u=sqrt (u2)
9  // results
10 printf (”root  mean  square  velocity  = %.2 e  cm/ sec ”,u)
```

Scilab code Exa 7.5 Example 5

```
1  clc
2  // Initialization  of  variables
3  n1 =2
4  n2 =10
5  n3 =3
6  P=720  //mm of  Hg
7  // calculations
8  n=n1+n2+n3
9  x1=n1/n
10 P1=x1*P
```

```
11  x2=n2/n
12  P2=x2*P
13  x3=n3/n
14  P3=x3*P
15  //results
16  printf("\n  Partial  pressure  of  N2 = %d  mm",P1)
17  printf("\n  Partial  pressure  of  O2 = %d  mm",P2)
18  printf("\n  Partial  pressure  of  CO2 = %d  mm",P3)
```

Scilab code Exa 7.6 Example 6

```
1   clc
2   //Initialization  of  variables
3   T=273.2+25  //K
4   n=1  //mol
5   R=1.987  //cal/deg  mol
6   //calculations
7   Etr=1.5*n*R*T
8   Erot=1.5*n*R*T
9   Evib=0
10  Eel=0
11  Etot=Etr+Erot+Evib+Eel
12  //results
13  printf("Total  energy = %d  cal",Etot)
```

Scilab code Exa 7.7 Example 7

```
1   clc
2   //Initialization  of  variables
3   b=24.1  //cm^2/mol
4   N=6.023*10^23  //mole^-1
5   //calculations
6   d=(3*b/(2*%pi*N))^(1/3)
```

```
7  // results
8  printf (" Molecular  diameter  of  He  =  %.2 e  cm" ,d)
```

Scilab code Exa 7.8 Example 8

```
1  clc
2  // Initialization  of  variables
3  P=100  // atm
4  T=200  //K
5  n=1  // mole
6  R=0.08206  // l  atm/deg  mol
7  disp (" From  psychrometric  charts ,")
8  Tc=126.2  //K
9  Pc=33.5  //K
10 // calculations
11 Pr=P/Pc
12 Tr=T/Tc
13 disp (" From  z  charts ,")
14 z=0.83
15 V=z*n*R*T/P
16 // results
17 printf (" Volume  =  %.3 f  liter" ,V)
```

Chapter 8

First law of thermodynamics

Scilab code Exa 8.1 Example 1

```scilab
1 clc
2 // Initialization of variables
3 P=1.0132*10^6 // dynes/cm^2
4 A=100 // cm^2
5 z=10 // cm
6 // calculations
7 w=P*A*z*10^-7
8 // results
9 printf("Joules = %.4e J",w)
```

Scilab code Exa 8.2 Example 2

```scilab
1 clc
2 // Initialization of variables
3 P=1.0132*10^6 // dynes/cm^2
4 A=100 // cm^2
5 z=10 // cm
6 // calculations
```

```
7  w=P*A*z*10^-7
8  cal=w/4.184
9  //results
10 printf(" Calories = %.3f cal",cal)
```

Scilab code Exa 8.3 Example 3

```
1  clc
2  //Initialization of variables
3  T=373.2 //K
4  n=1 //mol
5  qp=9720 //cal/mol
6  //calculations
7  q=n*qp
8  w=1.987*T
9  dE=q-w
10 //results
11 printf("Heat of vaporization = %d cal",q)
12 printf("\n Change in energy = %d cal",dE)
```

Scilab code Exa 8.4 Example 4

```
1  clc
2  //Initialization of variables
3  T1=25+273 //K
4  T2=25+273 //K
5  //calculations
6  disp("Since, T2=T1, dE=0")
7  dE=0
8  w=0
9  q=dE+w
10 //results
11 printf("\n Work done = %d ",w)
```

```
12  printf("\n Heat transferred = %d ",q)
13  printf("\n Change in energy = %d",dE)
```

Scilab code Exa 8.5 Example 5

```
1  clc
2  //Initialization of variables
3  R=1.987 //cal/deg mol
4  //calculations
5  Cvtr=1.5*R
6  Cvrot=1.5*R
7  Cvt=Cvtr+Cvrot
8  disp("Observed Cv= 6.43")
9  Cvobs=6.43
10 Cvvib=Cvobs-Cvt
11 //results
12 printf("Vibrational = %.2f cal/deg mol",Cvvib)
```

Chapter 9

Boltzmann distribution law

Scilab code Exa 9.1 Example 1

```scilab
1  clc
2  //Initialization of variables
3  r=2.1*10^-6  //cm
4  n=889
5  x=0.1  //cm
6  T=298.2  //K
7  //calculations
8  V=4/3 *%pi *r^3
9  rho=19.3-1
10 ffd=rho*V*980.7
11 eps=ffd*x
12 logN=-6.96*10^-14 /(2.303*1.38*10^-16 *T)
13 N=10^logN *n
14 //results
15 printf("No. of particles = %d ",N+1)
```

Scilab code Exa 9.2 Example 2

```
 1  clc
 2  //Initialization of variables
 3  x=1  //percent
 4  wave=1595  //cm^-1
 5  //calculations
 6  E=2.8593*wave
 7  Nratio=(100-x)/x
 8  logN=log10(Nratio)
 9  T=E/(2.303*1.987*logN)
10  //results
11  printf("Temperature = %d K",T)
```

Chapter 10

Second law of thermodynamics

Scilab code Exa 10.1 Example 1

```
1  clc
2  // Initialization of variables
3  T2=100+273.2 //K
4  T1=50+273.2 //K
5  n=1 //mol
6  R=1.987 //cal/deg mol
7  // calculations
8  dS=5/2 *n*R*2.303*log10(T2/T1)
9  // results
10 printf("Change in entropy = %.3f eu",dS)
```

Scilab code Exa 10.3 Example 3

```
1  clc
2  // Initialization of variables
3  H=380 //cal
4  T=273.2+32.1 //K
5  // calculations
```

```
6  dS=H/T
7  //results
8  printf("Entropy change = %.2f eu",dS)
```

Scilab code Exa 10.5 Example 5

```
 1  clc
 2  //Initialization of variables
 3  Ha=0
 4  Hb=0
 5  //calculations
 6  H=Ha+Hb
 7  q=H
 8  U=0
 9  w=q-H
10  //results
11  printf("Work done = %d",w)
```

Scilab code Exa 10.6 Example 6

```
1  clc
2  //Initialization of variables
3  prob=0.001
4  R=1
5  N=6.023*10^23
6  //calculations
7  dS=1.987*2.303*log10(prob) /N
8  //results
9  printf("change in entropy = %.1e eu",dS)
```

Scilab code Exa 10.7 Example 7

```
1 clc
2 //Initialization of variables
3 T=373.2 //K
4 c=1.987 //cal/deg
5 //calculations
6 w=c*T
7 A=-w
8 //results
9 printf("Change in A = %d cal",A)
```

Chapter 11

Condensed phases

Scilab code Exa 11.1 Example 1

```
1  clc
2  // Initialization of variables
3  A =7.6546
4  B =1686.8
5  T =60+273.2
6  // calculations
7  logP = A -B / T
8  P =10^ logP
9  // results
10 printf (" Vapor Pressure = %d mm " ,P +1)
```

Scilab code Exa 11.2 Example 2

```
1  clc
2  // Initialization of variables
3  alpha =4.92*10^ -5  // deg^ -1
4  beta =7.85*10^ -7  // atm^ -1
5  d =8.93  // g / cm^ 3
```

```scilab
 6  T =298.15  //K
 7  // calculations
 8  dC =63.54* T * alpha ^2 *1.987/( d * beta *82.06)
 9  // results
10  printf ("Change in c values = %.3 f cal/deg mol",dC)
```

Chapter 12

Physical Equilibria

Scilab code Exa 12.1 Example 1

```
1 clc
2 //Initialization of variables
3 p=3
4 c=2
5 //calculations
6 f=2-p+c
7 //results
8 printf("no. of degrees of freedom = %d ",f)
```

Scilab code Exa 12.2 Example 2

```
1 clc
2 //Initialization of variables
3 T=273.2 //K
4 vw=1.0001 //cm^3 /g
5 vi=1.0907 //cm^3 /g
6 hf=79.7 //cal/g
7 P1=76 //cm
```

```
 8  P2 =4.6  //cm
 9  // calculations
10  dT=T*( vw - vi ) *( P2 - P1 ) *13.6*980.7/( hf *4.184*10^7)
11  // results
12  printf (" change  in  temperature  =  %.4 f  deg " ,dT )
```

Scilab code Exa 12.3 Example 3

```
 1  clc
 2  // Initialization  of  variables
 3  V =6.84  //cm^3  /g
 4  // calculations
 5  dPbydT = -1.7*4.184*10^7  /(2.19* V *0.06*1.01*10^6)
 6  // results
 7  printf (" dPbydT  =  %d  atm/ deg " ,dPbydT )
```

Scilab code Exa 12.4 Example 4

```
 1  clc
 2  // Initialization  of  variables
 3  P =6   //atm
 4  T =273.2+25  //K
 5  P =23.8  //mm
 6  V =0.018  // lt /mol
 7  R =0.08206  // lt  am/ deg  mol
 8  // calculations
 9  dPa=V*P*4536/( R*T *760)
10  Pa=dPa+P
11  // results
12  printf (" Pressure  =  %.1 f  mm" ,Pa )
```

Scilab code Exa 12.5 Example 5

```scilab
1  clc
2  //Initialization of variables
3  x=0.25
4  Ps1=96 //mm
5  Ps2=43.9 //mm
6  //calculations
7  P1=x*Ps1
8  P2=(1-x)*Ps2
9  P=P1+P2
10 Xdash=P1/P
11 //results
12 printf("mole fraction of methanol in vapor = %.3f ",
        Xdash)
```

Scilab code Exa 12.6 Example 6

```scilab
1  clc
2  //Initialization of variables
3  Hv=539.6 //cal/g
4  T=273.2+100 //K
5  //calculations
6  Kb=1.987*T^2 /(1000*Hv)
7  //results
8  printf("Molal elevation constant = %.3f deg /mole /
        kg",Kb)
```

Scilab code Exa 12.7 Example 7

```scilab
1  clc
2  //Initialization of variables
3  ms=0.5 //mol/kg
```

```
4  m=5  //g
5  mw=100  //g
6  Ws=1000  //g/kg
7  //calculations
8  Ma=m*Ws/(ms*mw)
9  //results
10 printf("Molecular weight of solute = %d g/mol ",Ma)
```

Scilab code Exa 12.8 Example 8

```
1  clc
2  //Initialization of variables
3  dT=0.23  //C
4  Kb=1.86  //deg/mol/kg
5  //calculations
6  m=dT/Kb
7  //results
8  printf("molality of solution = %.2f m",m)
```

Scilab code Exa 12.9 Example 9

```
1  clc
2  //Initialization of variables
3  p=0.1  //m
4  T=30+273.2  //K
5  R=0.08206  //lt atm /deg/mol
6  P1=1  //atm
7  //calculations
8  w=1000/p
9  V=w/1000
10 dP=R*T/V
11 P=dP+P1
12 //results
```

```
13   printf (" Osmotic  Pressure =%.2 f  atm  " ,P)
```

Chapter 13

Thermodynamic changes accompanying chemical reaction

Scilab code Exa 13.1 Example 1

```
1 clc
2 // Initialization of variables
3 n1=10 // mol
4 n2=12 // mol
5 // calculations
6 dn=n1-n2
7 // results
8 printf("dHp = dEv- %d *RT",dn)
```

Scilab code Exa 13.2 Example 2

```
1 clc
2 // Initialization of variables
3 Ht1=-22063 // cal
```

```
4 T=298.15 //K
5 //calculations
6 H=Ht1 +0.5293*T + 0.3398*10^-3 *T^2 - 2.039*10^-7 *T
      ^3
7 //results
8 printf("Enthalpy = %d cal",H)
```

Scilab code Exa 13.3 Example 3

```
1 clc
2 //Initialization of variables
3 Cp=0.797 //cal/deg/mol
4 //calculations
5 S=Cp/3
6 //results
7 printf("Entropy = %.3f eu/mol",S)
```

Scilab code Exa 13.4 Example 4

```
1 clc
2 //Initialization of variables
3 T1=77.32 //K
4 P=1 //atm
5 T2=126 //K
6 Pc=33.5 //atm
7 //calculations
8 dS=27/32 *1.987*P/Pc *(T2/T1)^3
9 //results
10 printf("Change in entropy = %.2f eu/mol",dS)
```

Scilab code Exa 13.5 Example 5

```
1  clc
2  //Initialization of variables
3  S1=57.47
4  S2=50.34
5  S3=49
6  H1=8.09
7  H2=21.06
8  H3=0
9  F1=12.39
10 F2=20.72
11 F3=0
12 //calculations
13 dS=S1-S2-0.5*S3
14 dH=H1-H2-0.5*H3
15 dF=F1-F2-0.5*F3
16 //results
17 printf("Change in entropy = %.2f eu",dS)
18 printf("\n Change in enthalpy = %.2f kcal",dH)
19 printf("\n Change in free energy = %.2f kcal",dF)
```

Scilab code Exa 13.6 Example 6

```
1  clc
2  //Initialization of variables
3  P1=0.01
4  P2=0.1
5  P3=0.01
6  dF0=-54640  //cal
7  T=298.15  //K
8  R=1.987  //cal/deg
9  //calculations
10 Qp=P1/(P2*P3^0.5)
11 dF=dF0+R*T*log(Qp)
```

```
12  //results
13  printf("change in free energy = %d cal",dF)
```

Scilab code Exa 13.7 Example 7

```
1   clc
2   //Initialization of variables
3   disp("From table 13.4 ")
4   logKfwater=40.04724
5   logKfH2=0
6   logKfO2=0
7   //calculations
8   logK=logKfwater-logKfH2-0.5*logKfO2
9   K=10^logK
10  //results
11  printf("Equilibrium constant = %.4e",K)
```

Scilab code Exa 13.8 Example 8

```
1   clc
2   //Initialization of variables
3   Kp=1.1*10^40 //atm^-0.5
4   dn=-0.5
5   R=0.08206 //lt atm/deg mol
6   T=298.15 //K
7   //calculations
8   Kc=Kp*(R*T)^(-dn)
9   //results
10  printf("Kc = %.1e (mol/lt)^-0.5",Kc)
```

Scilab code Exa 13.9 Example 9

```
1  clc
2  //Initialization of variables
3  Kp=0.141 //atm
4  P=1 //atm
5  nu=2
6  R=0.08206 //lt atm/deg mol
7  T=298.15 //K
8  M=92.02 //g/mol
9  //calculations
10 a=poly(0,"a");
11 p=Kp*a^2 +4*a^2*P -Kp
12 z=roots(p)
13 alpha=z(1)
14 wbyV=P*M/(R*T*(1+(nu-1)*alpha))
15 //results
16 printf("Density of the equilibrium mixture = %.2f g/
       lt",wbyV)
```

Scilab code Exa 13.10 Example 10

```
1  clc
2  //Initialization of variables
3  x=0.5
4  P=0.468 //atm
5  //calculations
6  P1=x*P
7  P2=x*P
8  Kp=P1*P2
9  //results
10 printf("Final pressure after quilibrium = %.4f atm^2
       ",Kp)
```

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Chapter 14

Development and use of activity concepts

Scilab code Exa 14.1 Example 1

```
1 clc
2 // Initialization of variables
3 x1 =0.0200
4 Kx =812
5 // calculations
6 disp (" Neglecting 2x in comparision with x1 ,")
7 x = x1 / Kx
8 // results
9 printf (" Moles of Iodine present = %.2 e mole",x)
```

Scilab code Exa 14.2 Example 2

```
1 clc
2 // Initialization of variables
3 Kc =1.749*10^ -5 //M
4 n1 =0.1 // mole
```

```
5 n2 =0.01 // mole
6 // calculations
7 c = n1 / n2 * Kc
8 // results
9 printf (" Concentration of Hplus ions = %.1 e M" ,c)
```

Scilab code Exa 14.3 Example 3

```
1 clc
2 // Initialization of variables
3 c =0.01 //M
4 kc =1.749*10^ -5 //M
5 // calculations
6 x2 = c * kc
7 x = sqrt ( x2 )
8 // results
9 printf (" Concentraton of Hplus ions = %.1 e M" ,x)
```

Scilab code Exa 14.4 Example 4

```
1 clc
2 // Initialization of variables
3 K2 =1.0008*10^ -14 //m ^2
4 K1 =1.754*10^ -5 //m
5 c =0.1
6 // calculations
7 disp (" Neglecting x w.r.t c ,")
8 x2 = c * K2 / K1
9 x = sqrt ( x2 )
10 // results
11 printf (" Concentration of OH minus ions = %.1 e m" ,x)
```

Scilab code Exa 14.5 Example 5

```
1  clc
2  //Initialization of variables
3  disp("from table 14.1,")
4  r1=7.47*10^-5 //m
5  r2=4.57*10^-3 //m
6  mp=1.008*10^-14 //m^2
7  //calculations
8  r3=r2/r1
9  mH2=r3*mp
10 mH=sqrt(mH2)
11 //results
12 printf("Concentraton of Hplus ions = %.2e M",mH)
```

Scilab code Exa 14.6 Example 6

```
1  clc
2  //Initialization of variables
3  disp("from table 14.1,")
4  r1=1.75*10^-5 //m
5  r2=1.772*10^-4 //m
6  mp=1.008*10^-14 //m^2
7  //calculations
8  r3=r2/r1
9  mH2=r3*mp
10 mH=sqrt(mH2)
11 //results
12 printf("Concentraton of Hplus ions = %.1e M",mH)
```

Scilab code Exa 14.7 example 7

```
1  clc
2  //Initialization of variables
3  c=1*10^-6 //m
4  K=1.754*10^-5 //m
5  Kp=1.008*10^-14 //m^2
6  //calculations
7  mH=c
8  //Iteration 1
9  mOH=Kp/mH
10 mA=mH-mOH
11 mHA=mH*mA/K
12 mH2=mH-mHA+mOH
13 //Iteration 2
14 mOH2=Kp/mH2
15 mA2=mH2-mOH2
16 mHA2=mH2*mA2/K
17 mH3=mH2-mHA2+mOH2
18 //From x2
19 x2=sqrt(Kp)
20 x1=c
21 mOH3=Kp/x2
22 y2=x1
23 //From x1
24 mOH4=Kp/c
25 mA4=mH-mOH4
26 mHA4=mH*mA4/K
27 y1=c-mHA4-mA4
28 //upon further iterations, we get
29 mHplus=mH3
30 //results
31 printf("Concentration of H plus ions = %.2e m",
       mHplus)
32 //The answer is a bit different due to rounding off
       error.
```

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Scilab code Exa 14.8 Example 8

```scilab
1  clc
2  //Initialization of variableH
3  disp("From table 14-3,")
4  HH=0
5  HHcoo=-98
6  HHcooh=-98
7  SH=0
8  SHcoo=21.9
9  SHcooh=39.1
10 KH=0
11 KHcoo=58.64
12 KHcooh=62.38
13 //calculationH
14 dH=HH+HHcoo-HHcooh
15 dS=SH+SHcoo-SHcooh
16 dK=KH+KHcoo-KHcooh
17 K=10^dK
18 //results
19 printf(" dS0 = %.1f eu",dS)
20 printf("\n dH0 = %.1f kcal",dH)
21 printf("\n log Krm = %.2f ",dK)
22 printf("\n Krm = %.1e m",K)
```

Scilab code Exa 14.9 Example 9

```scilab
1  clc
2  //Initialization of variables
3  mca=0.01 //m
4  mcl=0.02 //m
5  //calculations
```

```
6  Mu=0.5*(mca*4 + mcl*1)
7  disp("From table 14-5,")
8  aca=6 //A
9  acl=3 //A
10 disp("From table 14-6,")
11 gaca=0.555
12 gacl=0.843
13 Aca=gaca*mca
14 Acl=gacl*mcl
15 //results
16 printf("Activity of cl = %.4f ",Acl)
17 printf("\n Activity of ca = %.4f ",Aca)
```

Scilab code Exa 14.10 Example 10

```
1  clc
2  //Initialization of variables
3  m1=0.1 //m
4  m2=0.1 //m
5  K=1.754*10^-5 //m
6  //calculations
7  mu=0.5*(m1*1^2 + m2*1^2)
8  disp("From table 14.5,")
9  aH=9 //A
10 aA=4.5 //A
11 disp("From table 14.6")
12 gH=0.825
13 gA=0.775
14 gHA=1
15 x1=gHA*K/(gH*gA)
16 disp("Assuming x to be small w.r.t m1,")
17 x=sqrt(x1*m1)
18 //results
19 printf("Concentration of H plus ions = %.2e m",x)
```

Scilab code Exa 14.11 Example 11

```
1  clc
2  //Initialization of variables
3  K=1.754*10^-5  //m
4  c=0.1
5  //calculations
6  disp("Neglecting x w.r.t c,")
7  x2=K
8  x=sqrt(K)
9  mu=x
10 disp("From tables 14-5 and 14-6,")
11 gH=0.963
12 gA=0.960
13 x22=K/(gH*gA)
14 a=poly(0,"a");
15 p=a^2 +a*x22 -c*x22
16 z=roots(p)
17 alpha=z(2)
18 //results
19 printf("concentration of H plus ions = %.2e m",alpha
       )
```

Scilab code Exa 14.12 Example 12

```
1  clc
2  //Initialization of variables
3  disp("From table 14.3")
4  K1=-13.5089
5  K2=-22.9792
6  K3=19.2218
7  c=0.1  //m
```

```
 8  //calculations
 9  logK=K1-K2-K3
10  K=10^logK
11  mu=0.5*(c*1^2 + c*1^2)
12  disp("From tables 14-5 and 14-6,")
13  gAg=0.745
14  gCl=0.755
15  x2=K/(gAg*gCl)
16  x=sqrt(x2)
17  //results
18  printf("Solubility of Agcl = %.2e m",x)
```

Scilab code Exa 14.13 Example 13

```
 1  clc
 2  //Initialization of variables
 3  Cna=0.11
 4  Ccl=0.1
 5  //calculations
 6  x=poly(0,"x");
 7  p=99*x^2 - 2.1*x+Cna*Ccl
 8  z=roots(p)
 9  alpha=z(2)
10  Na1=Cna-10*alpha
11  Cl1=Ccl-10*alpha
12  //results
13  printf(" Concentration of Na in 1  = %.4f M',Na1)
14  printf("\n Concentration of Cl in 1  = %.4f M',Cl1)
15  printf("\n Concentration of Na in 2  = %.4f M',alpha
        )
16  printf("\n Concentration of Cl in 2  = %.4f M',alpha
        )
```

Chapter 15

Electrochemistry

Scilab code Exa 15.1 Example 1

```
1  clc
2  // Initialization of variables
3  I=0.5   //amp
4  t=55    //min
5  we=31.77
6  // calculations
7  Q=I*t*60
8  n=Q/96496
9  w=n*we
10 // results
11 printf(" Weight of copper leaving = %.3f g",w)
```

Scilab code Exa 15.2 Example 2

```
1  clc
2  // Initialization of variables
3  w1=0.7532  //g
4  w2=0.9972  //g
```

```
5  wdep=0.4  //g
6  we=31.77  //g
7  //calculations
8  dn=w2/we - w1/we
9  t=dn/(wdep/we)
10 dne=wdep/we
11 dnmig=dn-dne
12 tplus=-dnmig/dne
13 tminus=1-tplus
14 //results
15 printf("tplus  = %.3f",tplus)
16 printf("\n tminus= %.3f",tminus)
```

Scilab code Exa 15.3 Example 3

```
1  clc
2  //Initialization of variables
3  R1=312  //ohms
4  R2=1043  //ohms
5  c=0.01  //N
6  kdash=0.002768  //ohm^-1cm^-1
7  //calculations
8  k=kdash*R1
9  kdash2=k/R2
10 lambda=kdash2/(c/1000)
11 //results
12 printf("Equivalent  conductance  = %.1f ohm^-1  cm^2
      equiv^-1",lambda)
```

Scilab code Exa 15.4 Example 4

```
1  clc
2  //Initialization of variables
```

```
3  l1 =349.8
4  l2 =40.9
5  // calculations
6  l= l1 + l2
7  // results
8  printf ("Conductance for acetic acid = %.1 f ohm^−1 cm
      ^2",l)
```

Scilab code Exa 15.5 Example 5

```
1  clc
2  // Initialization of variables
3  l1 =63.6
4  l2 =79.8
5  n=1  // mg/lt
6  we =116.7 // g/equiv
7  // calculations
8  l= l1 + l2
9  c= n *10^ -3 / we
10 k= c * l /1000
11 // results
12 printf (" Specific conductance = %.2 e ohm^−1 cm^−1",k)
```

Scilab code Exa 15.6 Example 6

```
1  clc
2  // Initialization of variables
3  e1 =0.763 // volt
4  e2 =0.337 // volt
5  // calculations
6  e0 = e1 + e2
7  // results
```

```
8  printf("Standard electrode potential of the cell = %
      .3 f volts",e0)
```

Scilab code Exa 15.7 Example 7

```
1  clc
2  //Initialization of variables
3  aZn =0.1
4  aCu =0.01
5  e1 =0.763 // volt
6  e2 =0.337 // volt
7  //calculations
8  e0 = e1 + e2
9  Q = aZn / aCu
10 E = e0 - 0.05915* log10 (Q) /2
11 //results
12 printf ("Emf of the cell = %.3 f volts",E)
```

Chapter 16

Typical mechanisms and rate laws

Scilab code Exa 16.1 Example 1

```
1 clc
2 // Initialization of variables
3 P1 =69.2 //mm
4 P2 =39.8 //mm
5 t =20 //min
6 // calculations
7 k =2.303* log10 (P1/P2) /(t*60)
8 // results
9 printf ("Rate constant = %.2e sec^-1",k)
```

Scilab code Exa 16.2 Example 2

```
1 clc
2 // Initialization of variables
3 t =10 //min
4 x =90
```

```
5 // calculations
6 k=2.303* log10 (100/(100 -x)) /t
7 // results
8 printf ("Rate constant = %.3 f min^-1",k)
```

Scilab code Exa 16.3 Example 3

```
1 clc
2 // Initialization of variables
3 t=242 // sec
4 P=229 //mm
5 P0=363 //mm
6 // calculations
7 k=(1/P -1/P0)/t
8 // results
9 printf ("rate constant= %.2 e sec^-1 mm^-1",k)
```

Chapter 17

Resolving Kinetic data

Scilab code Exa 17.1 Example 1

```
1  clc
2  //Initialization of variablesx1=5
3  x2=20
4  x1=5
5  n1=7.49
6  n2=5.14
7  //calculations
8  n=(log(n1)-log(n2))/(log(100-x1) - log(100-x2))
9  //results
10 printf("Order of the reaction  = %.2f",n)
```

Scilab code Exa 17.2 Example 2

```
1  clc
2  //Initialization of variables
3  p2=169
4  p1=363
5  t1=410
```

```
6  t2=880
7  //calculations
8  ndash=(log(t2) - log(t1))/(log(p1) - log(p2))
9  n=ndash+1
10 //results
11 printf("Order of the reaction = %.2f",n)
```

Scilab code Exa 17.3 Example 3

```
1  clc
2  //Initialization of variables
3  R=1.987 //cal/deg/mol
4  k1=4.45*10^-5
5  k2=2.52*10^-6
6  T1=283+273.2 //K
7  T2=356+273.2 //K
8  //calculations
9  Ea=2.303*R*1.7530 /(1/T1 - 1/T2)
10 logZ= log10(k1) +Ea/(2.303*R*T1)
11 Z=10^logZ
12 //results
13 printf("Activation energy = %d cal/mol",Ea)
14 printf("\n Z = %.1e lt /mol sec",Z)
```

Scilab code Exa 17.5 Example 5

```
1  clc
2  //Initialization of variables
3  g1=0.661
4  g2=0.899
5  g3=0.405
6  g4=0.803
7  g5=0.946
```

```
 8  g6 =0.614
 9  k =1.33
10  // calculations
11  k0=k*g3/(g1*g2)
12  k2=k0*g4*g5/g6
13  // results
14  printf ("Equlibrium  constant = %.2 f  lt /mol  min",k2)
```

Chapter 18

Catalysis

Scilab code Exa 18.1 Example 1

```
1  clc
2  // Initialization  of  variables
3  V1 =0.284  // cm^3 /g
4  V2 =1.43  // cm^3 /g
5  P1 =142.4  // mm
6  P2 =760  // mm
7  // calculations
8  z =(1/ V1  -  1/ V2 )/(1/ P1  -  1/ P2 )
9  invVm =1/ V2  -  z/ P2
10 Vm =1/ invVm
11 // results
12 printf ( " Volume  =  %.1 f  cm^3/ g " , Vm )
13 // The  answer  in  the  textbook  is  a  bit  different  due
        to  rounding  off  error .
```

Scilab code Exa 18.2 Example 2

```
1  clc
```

```
2  //Initialization of variables
3  Vm=2.86 //cc/g
4  P=1 //atm
5  R=82.06 //cm^3 atm/deg mol
6  T=273.2 //deg
7  N=6.023*10^23
8  sigma=16.2*10^-16 //cm^2 /molecule
9  //calculations
10 n=P*Vm/(R*T)
11 A=N*n*sigma
12 //results
13 printf("total area = %.2e cm^2 (g catalyst)^-1",A)
```

Chapter 19

Photochemistry

Scilab code Exa 19.1 Example 1

```
1  clc
2  // Initialization  of  variables
3  r1=0.727
4  r2=0.407
5  // calculations
6  r3=r1*r2
7  // results
8  printf("Overall  transmittance  = %.3f",r3)
```

Scilab code Exa 19.2 Example 2

```
1  clc
2  // Initialization  of  variables
3  r=0.450
4  c=0.02  //M
5  l=4  //cm
6  // calculations
7  e=-log10(r) /(c*l)
```

```
8  // results
9  printf("Extinction coefficient = %.2f litres mole^-1
       cm^-1",e)
```

Scilab code Exa 19.3 Example 3

```
1  clc
2  //Initialization of variables
3  r1=0.850
4  r2=0.50
5  //calculations
6  Da=-log10(r1)
7  Db=-log10(r2)
8  D=Da+Db
9  r3=10^(-D)
10 //results
11 printf("Transmittance of solution = %.3f ",r3)
```

Scilab code Exa 19.4 Example 4

```
1  clc
2  //Initialization of variables
3  c=0.000025 //M
4  l=2 //cm
5  D=0.417
6  //calculations
7  e=D/(c*l)
8  //result
9  printf("Extinction coefficient = %d liters mole^-1
       cm^-1",e)
```

Scilab code Exa 19.5 Example 5

```scilab
1  clc
2  //Initialization of variables
3  c=0.5 //M
4  c1=0.000025 //M
5  D2=0.280
6  D1=0.417
7  //calculations
8  c2=D2*c1/(D1)
9  dC=c1-c2
10 SCN=c- 6*c2 -4*dC
11 K=dC*SCN^2 /c2
12 //results
13 printf("Kc for dissociation = %.2f M^2",K)
```

Scilab code Exa 19.6 Example 6

```scilab
1  clc
2  //Initialization of variables
3  D2=0.249
4  D1=0.172
5  a2=0.00752
6  a1=0.00527
7  //calculations
8  m=(log(D2) -log(D1))/(log(a2) - log(a1))
9  //results
10 printf("m = %.2f ",m)
```

Scilab code Exa 19.7 Example 7

```scilab
1  clc
2  //Initialization of variables
```

```
3  c = 0.1  //M
4  V = 100  //ml
5  v1 = 25  //ml
6  D = 0.980
7  d1 = 0.090
8  d2 = 0.150
9  // calculations
10  a = v1 * c / V
11  b = ( V - v1 ) * c / V
12  Da = a * d1 / c
13  Db = b * d2 / c
14  Ddash = Da + Db
15  dD = D - Ddash
16  // results
17  printf (" Increase  in  optical  density  = %.3 f ",dD)
```

Scilab code Exa 19.8 Example 8

```
1  clc
2  // Initialization  of  variables
3  E = 50000  // cal / mol
4  // calculations
5  lam = 2.8593 / E
6  // results
7  printf (" For  the  reaction  to  occur  lambda < %d A ",lam
      *10^8)
```

Scilab code Exa 19.9 Example 9

```
1  clc
2  // Initialization  of  variables
3  lam = 3000 * 10^-8  //cm
4  yield = 0.420
```

```
5  Et =70000 // cal
6  // calculations
7  E=2.8593/ lam
8  n=yield*Et/E
9  // results
10 printf("Amount of reactant disappeared = %.3f mol",n
      )
```