

R Textbook Companion for
Modern Physical Chemistry: A Molecular
Approach
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Book Description

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R 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)

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

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Chapter 1

Structure in Solids

R code Exa 1.1 Finding angle phi

```
1 # Page No. 3
2
3 n <- 1
4 lambda <- 0.70*10^-8
5 d <- 1/200
6 mins <- 5
7 mins_deg <- 60
8 radian <- 3.1416
9
10 theta <- (mins*radian)/(mins_deg*180)
11 phi <- sqrt(((n * lambda * 2) / d) + theta^2)
12
13 print(theta)
14 print(phi)
```

R code Exa 1.2 Finding interplanar spacing

```
1 # Page No. 6
```

```
2
3 library(pracma)
4
5 n <- 1
6 lambda <- 1.539
7 theta <- deg2rad(37.25)
8
9 d <- lambda / (2 * sin(theta))
10
11 print(d)
```

R code Exa 1.6 Calculating Avogadros number

```
1 # Page No. 17
2
3 n <- 4
4 rho <- 2.640
5 V <- 4.016*10^-8
6 M <- 25.939
7
8 m <- (rho * (V)^3) / n
9 N_a <- M / m
10
11 print(m)
12 print(N_a)
```

Chapter 2

Structure in Molecules and Atoms

R code Exa 2.1 Relation of homogeneous electron beam to the voltage accelerating the electrons

```
1 # Page No. 26
2
3 h <- 6.6261*10^-34
4 m <- 9.1094*10^-31
5 e <- 1.6022*10^-19
6
7 lambda <- h/sqrt(2*m*e)
8
9 print(lambda)
10 cat(lambda, "/V^(1/2)", sep = " ")
```

R code Exa 2.3 Calculating cross section presented by cadmium atom to beam

```
1 # Page No. 32
```

```
2
3 x <- 0.083
4 A <- 6.02*10^23
5 m <- 8.642
6 M <- 112.41
7 I <- 1*10^-4
8
9 n <- (m / M) * A
10 sigma <- -log(I) / (n * x)
11
12 print(n)
13 print(sigma)
```

Chapter 3

Gases and Collective Properties

R code Exa 3.2 Finding newtons per square meter in 1 atmosphere

```
1 # Page No. 40
2
3 g <- 9.80665
4 h <- 0.7600
5 m <- 13595.1
6
7 P <- g * h * m
8
9 print(P)
```

R code Exa 3.3 Calculating joules in 1 liter atmosphere

```
1 # Page No. 40
2
3 P <- 101325
4 v <- 10^3
5 Mu <- 10^-2
6
```

```
7 V <- v * (Mu^3)
8 J <- P * V
9
10 print(V)
11 print(J)
```

R code Exa 3.4 Changing the energy unit in R

```
1 # Page No. 43
2
3 r <- 8.31451
4 c <- 0.1
5 cal <- 4.18400
6
7 R <- r / c
8 R_1 <- r / cal
9
10 print(R)
11 print(R_1)
```

R code Exa 3.5 Calculating root mean square velocity of helium molecule

```
1 # Page No. 43
2
3 R <- 8.31451
4 T <- 293.15
5 M <- 0.0040026
6
7 u <- sqrt((3 * R * T) / M)
8
9 print(u)
```

R code Exa 3.6 Calculating the partial pressure

```
1 # Page No. 44
2
3 n <- 15
4 P <- 720
5 n_1 <- 2
6 n_2 <- 10
7 n_3 <- 3
8
9 P_N2 <- (n_1 / n) * P
10 P_O2 <- (n_2 / n) * P
11 P_CO2 <- (n_3 / n) * P
12
13 print(P_N2)
14 print(P_O2)
15 print(P_CO2)
```

R code Exa 3.7 Estimating energy associated with thermal agitation in 1 mole water vapour

```
1 # Page No. 46
2
3 n <- 1
4 R <- 8.31451
5 T <- 298.151
6 E_vib <- 0
7 E_el <- 0
8
9 E_tr <- 1.5 * n * R * T
10 E_rot <- 1.5 * n * R * T
11 E <- E_tr + E_rot + E_vib + E_el
```



```
12
13 print(E_tr)
14 print(E_rot)
15 print(E)
16
17 # The answer may slightly vary due to rounding off
    values.
```

R code Exa 3.8 Calculating radius of helium atom

```
1 # Page No. 48
2
3 b <- 24.1
4 pi <- 3.1416
5 N <- 6.022 * 10^23
6
7 r <- ((3 * b)/(16 * pi * N))^(1/3)
8
9 print(r)
```

R code Exa 3.9 Calculating number of particles in 32 layers of gold sol

```
1 # Page No. 54
2
3 pi <- 3.1416
4 r <- 4.5 * 10^-7
5 p <- 18.3
6 g <- 9.807
7 d <- 1000
8 h <- 0.200 * 10^-2
9 N_0 <- 89
10 k <- 1.3807 * 10^-23
11 T <- 298.15
```

```

12
13 V <- (4/3) * pi * (r^3)
14 F <- (p / d) * g * V
15 E <- F * h
16 N_1 <- exp(-E / (k * T))
17 N <- N_1 * N_0
18
19 print(V)
20 print(F)
21 print(E)
22 print(N_1)
23 print(N)
24
25 # The answer may slightly vary due to rounding off
    values.

```

R code Exa 3.13 Calculating cross section and mean relative speed and collision rate density for molecular oxygen

```

1 # Page No. 59
2
3 pi <- 3.1416
4 r <- 3.61 * 10^-10
5 R <- 8.31451
6 T <- 298.15
7 M <- 31.999 * 10^-3
8 k <- 1.3807 * 10^-23
9 P <- 1 * 10^5
10
11 alpha <- pi * (r^2)
12 v <- sqrt((16 * R * T) / (pi * M))
13 d <- P / (k * T)
14 Z <- 0.5 * alpha * v * (d^2)
15
16 print(alpha)

```

```
17 print(v)
18 print(d)
19 print(Z)
```

R code Exa 3.14 Calculating hypothetical maximum specific reaction rate

```
1 # Page No. 59
2
3 a <- 4.094 * 10^-19
4 v <- 628.1337
5 N_a <- 6.022 * 10^23
6
7 k_aa <- 0.5 * a * v * N_a * 1000
8
9 print(k_aa)
```

Chapter 4

The First Law for Energy

R code Exa 4.3 Calculating delta E and delta H for vaporization of 1 mole water

```
1 # Page No. 69
2
3 h <- 40893
4 mol <- 1
5 R <- 8.31451
6 T <- 372.778
7
8 q <- mol * h
9 w <- -R * T
10 E <- q + w
11 H <- q
12
13 print(E)
14 print(H)
```

R code Exa 4.5 Calculating w and delta E and q for the overall process

```
1 # Page No. 72
2
3 w <- 0
4 E <- 0
5
6 q <- E - w
7
8 print(q)
```

R code Exa 4.6 Estimating translational and rotational and vibrational contributions

```
1 # Page No. 75
2
3 R <- 8.31451
4 Cv_500 <- 26.90
5
6 Cv_tr <- 3 * R / 2
7 Cv_rot <- 3 * R / 2
8 Cv_vib <- Cv_500 - (Cv_tr + Cv_rot)
9
10 print(Cv_rot)
11 print(Cv_tr)
12 print(Cv_vib)
```

Chapter 5

Entropy and the Second Law

R code Exa 5.1 Calculating entropy change

```
1 # Page No. 89
2
3 q <- 1590
4 C <- 32.1
5
6 T <- C + 273
7 S <- q / T
8
9 print(S)
```

R code Exa 5.2 Calculating entropy change

```
1 # Page No. 89
2
3 n <- 1
4 R <- 8.31451
5 T1 <- 323.15
6 T2 <- 373.15
```

```
7
8 S <- 2.5 * n * R * log(T2/T1)
9
10 print(S)
```

R code Exa 5.4 Calculating entropy change

```
1 # Page No. 93
2
3 w <- 0.001
4 k <- 1.3807 * 10^-23
5
6 S <- k * log(w)
7
8 print(S)
```

R code Exa 5.5 Finding delta A and G for vaporization of 1 mole water

```
1 # Page No. 96
2
3 w <- -3099
4
5 A <- q + w - q
6 G <- q - q
7
8 print(A)
9 print(G)
```

R code Exa 5.8 Calculating the thermodynamic force acting on a solute

```
1 # Page No. 101
2
3 x <- 10
4 c <- log(2)
5 R <- 8.31451
6 T <- 298.15
7
8 a <- c / x
9 F <- (R * T * c * 100) / x
10
11 print(F)
```

R code Exa 5.9 Determining the gravitational force

```
1 # Page No. 102
2
3 M <- 0.100
4 g <- 9.807
5
6 F <- -M * g
7
8 print(F)
```

Chapter 6

Relationships between Phases

R code Exa 6.2 Determining endothermicity which causes a solution to separate into two phases

```
1 # Page No. 112
2
3 n <- 2
4 R <- 8.31451
5 C <- 40
6 X_a <- 0.5
7 X_b <- 0.5
8
9 T <- C + 273.15
10 q <- -n * R * T * (X_a * log(X_a) + X_b * log(X_b))
11
12 print(q)
13
14 # The answer may slightly vary due to rounding off
    values.
```

R code Exa 6.3 Calculating the change in melting point of ice

```

1 # Page No. 122
2
3 T1 <- 273.15
4 V <- -0.0906
5 L <- 333.5
6 j <- 0.101325
7 P1 <- 760
8 P2 <- 4.6
9
10 P <- ((P2 - P1) / P1) * j
11 T <- (T1 * V * P) / L
12
13 print(P)
14 print(T)

```

R code Exa 6.4 Calculating the vapour pressure of benzene

```

1 # Page No. 124
2
3 T <- 333.15
4 C <- 17.6254
5 slope <- 3884
6
7 P <- exp((-slope / T) + C)
8
9 print(P)

```

R code Exa 6.5 Determining partial pressure of water in saturated gas

```

1 # Page No. 125
2
3 R <- 0.08206
4 T <- 298.15

```

```

5 P_A <- 23.8
6 V <- 0.018
7 pp <- 6
8 P_a <- 760
9
10 P_1 <- pp - (P_A / P_a)
11 P <- (V * P_A * P_1) / (R * T)
12 final_P <- P + P_A
13
14 print(P_1)
15 print(P)
16 print(final_P)

```

R code Exa 6.6 Finding initial concentration of methanol in vaporu

```

1 # Page No. 127
2
3 X_A <- 0.250
4 X_B <- 0.750
5 VP_CH3OH <- 96
6 VP_C2H5OH <- 43.9
7
8 PCH3OH <- X_A * VP_CH3OH
9 PC2H5OH <- X_B * VP_C2H5OH
10 P <- PC2H5OH + PCH3OH
11 X_CH3OH <- PCH3OH / P
12
13 print(PC2H5OH)
14 print(PCH3OH)
15 print(X_CH3OH)

```

R code Exa 6.7 Calculating the molal elevation constant for water

```
1 # Page No. 130
2
3 R <- 8.31451
4 T <- 372.78
5 L <- 40671
6 M <- 18.015
7
8 K_b <- (R * (T^2) * M) / (L * 1000)
9
10 print(K_b)
```

R code Exa 6.8 Calculating osmotic pressure for a sucrose solution

```
1 # Page No. 135
2
3 M <- 0.100
4 C <- 30
5 R <- 0.08206
6
7 T <- C + 273.15
8 w <- 1000 / M
9 V <- w / 1000
10 P <- (R * T) / V
11
12 print(P)
```

Chapter 7

Relationships among Reactants

R code Exa 7.2 Determining delta H for a reaction

```
1 # Page No. 144
2
3 H_eqn1 <- -241.83
4 H_eqn2 <- -136.11
5
6 H_eqn <- (2 * -H_eqn1) + H_eqn2
7
8 print(H_eqn)
```

R code Exa 7.5 Calculating entropy correction for gas imperfection

```
1 # Page No. 150
2
3 R <- 8.31451
4 P <- 1.000
5 P_c <- 33.9
6 T_c <- 126
7 T <- 77.32
```

```
8
9 S <- (27 / 32) * R * (P / P_c) * ((T_c / T)^3)
10
11 print(S)
```

R code Exa 7.6 Calculating delta S and G and H

```
1 # Page No. 151
2
3 S_NO2 <- 240.02
4 S_NO <- 210.76
5 S_O2 <- 205.15
6 H_NO2 <- 33.10
7 H_NO <- 90.29
8 H_O2 <- 0
9 G_NO2 <- 51.26
10 G_NO <- 86.60
11 G_O2 <- 0
12
13 S <- S_NO2 - S_NO - (0.5 * S_O2)
14 H <- H_NO2 - H_NO - (0.5 * H_O2)
15 G <- G_NO2 - G_NO - (0.5 * G_O2)
16
17 print(S)
18 print(G)
19 print(H)
```

R code Exa 7.7 Calculating Gibbs energy change

```
1 # Page No. 155
2
3 P_H2O <- 0.0500
4 P_H2 <- 0.0100
```

```

5 P_O2 <- 0.1000
6 G_o <- -228.62
7 R <- 8.31451
8 T <- 298.15
9
10
11 Q <- P_H2O / (P_H2 * sqrt(P_O2))
12 G <- G_o + (R * 10^-3 * T * log(Q))
13
14 print(Q)
15 print(G)

```

R code Exa 7.8 Determining the equilibrium constant

```

1 # Page No. 156
2
3 Kf_H2O <- 40.053
4 Kf_H2 <- 0
5 Kf_O2 <- 0
6
7 log_K <- (Kf_H2O) - Kf_H2 - (0.5 * Kf_O2)
8 K <- 10^log_K
9
10 print(log_K)
11 print(K)

```

R code Exa 7.9 Calculating Kp and Kc

```

1 # Page No. 159
2
3 R <- 0.083145
4 C <- 25
5 K_p <- 1.130 * 10^40

```

```

6 n <- -1/2
7
8 T <- C + 273.15
9 K <- K_p * (R * T)^-n
10
11 print(K)

```

R code Exa 7.11 Calculating Kp

```

1 # Page No. 160
2
3 K_N2O4 <- -17.132
4 K_NO2 <- -8.981
5
6 K <- 10^((2 * (K_NO2)) - (K_N2O4))
7
8 print(K)

```

R code Exa 7.12 Calculating the density of an equilibrium mixture

```

1 # Page No. 160
2
3 w <- 0.148
4 P <- 1
5 M <- 92.011
6 R <- 0.083145
7 T <- 298.15
8 v <- 2
9
10 a <- sqrt(w / (4 + w))
11 rho <- (P * M) / (R * T * (1 + ((v - 1) * a)))
12
13 print(a)

```



```
14 print(rho)
```

R code Exa 7.13 Calculating final pressure after equilibrium

```
1 # Page 161
2
3 library(polynom)
4
5 kp <- 0.0562
6 ml <- 0.5
7
8 x <- solve(polynomial(c(-kp,0.5,1)))[solve(
  polynomial(c(-kp,0.5,1))>0]
9
10 print(x+kp/x)
```

Chapter 8

Equilibria in Condensed Phases

R code Exa 8.1 Calculating amount of I2 in equilibrium

```
1 # Page No. 174
2
3 library(Ryacas)
4
5 mol <- 0.0200
6 MF <- 812
7 n <- yac_symbol("n")
8
9 x <- eval(yac_expr(simplify(mol / (((MF * n) / n) +
10     2))))
11 print(x)
```

R code Exa 8.2 Calculating hydrogen ion concentration in a solution

```
1 # Page No. 175
2
3 K <- 1.749 * 10^-5
```

```

4 C_CH3COOH <- 0.100
5 C_CH3COO <- 0.0100
6
7 C_H <- (C_CH3COOH / C_CH3COO) * K
8
9 print(C_H)

```

R code Exa 8.3 Calculating hydrogen ion concentration

```

1 # Page No. 175
2
3 library(polynom)
4
5 Kc <- 1.749 * 10^-5
6 M <- 0.0100
7
8 k <- M * Kc
9 x <- solve(polynomial(c(-k,Kc,1)))[solve(polynomial(
    c(-k,Kc,1))>0]
10
11 print(x)

```

R code Exa 8.4 Calculate the hydroxide ion concentration

```

1 # Page No. 176
2
3 K <- 1.749 * 10^-5
4 K_m <- 1.008 * 10^-14
5 m_CH3COOH <- x
6 m_CH3COO <- 0.100
7
8 x <- sqrt((m_CH3COO * K_m) / K)
9

```

```
10 print(x)
```

R code Exa 8.5 Calculating mH

```
1 # Page No. 179
2
3 m_1 <- 7.47 * 10^-5
4 m_2 <- 4.57 * 10^-3
5 mH_mOH <- 1.008 * 10^-14
6
7 MH_MOH <- m_2 / m_1
8 mH <- sqrt(mH_mOH * MH_MOH)
9
10 print(mH)
```

R code Exa 8.6 Calculating mH

```
1 # Page No. 180
2
3 m_1 <- 1.75 * 10^-5
4 m_2 <- 1.772 * 10^-4
5 mH_mOH <- 1.008 * 10^-14
6
7 MH_MOH <- m_2 / m_1
8 mH <- sqrt(mH_mOH * MH_MOH)
9
10 print(mH)
```

R code Exa 8.8 Finding delta H and delta S and K

```

1 # Page No. 183
2
3 S_H <- 0
4 S_HCOO <- 92
5 S_HCOOH <- 163
6 H_H <- 0
7 H_HCOO <- -425.55
8 H_HCOOH <- -425.43
9 logKf_H <- 0
10 logKf_HCOO <- 61.49
11 logKf_HCOOH <- -65.22
12
13 S <- S_H + S_HCOO - S_HCOOH
14 H <- H_H + H_HCOO - H_HCOOH
15 K <- 10^(logKf_H + logKf_HCOO + logKf_HCOOH)
16
17 print(S)
18 print(H)
19 print(K)
20
21 # The answer provided in the textbook is wrong.

```

R code Exa 8.9 Calculating hydrogen ion concentration

```

1 # Page No. 191
2
3 library(polynom)
4
5 K <- 1.754 * 10^-5
6 Y_HA <- 1
7 m_Na <- 0.100
8 z_Na <- 1
9 m_Cl <- 0.100
10 z_Cl <- 1
11 Y_H <- 0.825

```

```

12 Y_A <- 0.775
13 K_1 <- 2.743 * 10^-6
14
15 k <- (Y_HA / (Y_A * Y_H)) * K
16 x <- solve(polynomial(c(-K_1,k,1)))[solve(polynomial
      (c(-K_1,k,1)))>0]
17
18 print(x)

```

R code Exa 8.10 Calculating hydrogen ion concentration

```

1 # Page No. 194
2
3 library(polynom)
4
5 K <- 1.754 * 10^-5
6 Y_HA <- 1
7 Y_H <- 1
8 Y_A <- 1
9
10 K_3 <- (Y_HA / (Y_H * Y_A)) * K
11 x <- solve(polynomial(c(-K_3 / 10,K_3,1)))[solve(
      polynomial(c((-K_3 / 10),K_3,1)))>0]
12
13 Y2_H <- 0.963
14 Y2_A <- 0.961
15
16 k <- (Y_HA / (Y2_A * Y2_H)) * K
17 X <- solve(polynomial(c(-k / 10,k,1)))[solve(
      polynomial(c((-k / 10),k,1)))>0]
18
19 print(K_3)
20 print(x)
21 print(k)
22 print(X)

```

R code Exa 8.11 Calculating the solubility of AgCl

```
1 # Page No. 195
2
3 library(polynom)
4
5 K <- 1.768 * 10^-10
6 Y_Cl <- 0.755
7 Y_Ag <- 0.745
8 MM <- 143.321
9
10 K_1 <- (1 / (Y_Cl * Y_Ag)) * K
11 x <- sqrt(K_1)
12 w <- x * MM
13
14 print(x)
15 print(w)
16
17 # The answer provided in the textbook is wrong.
```

R code Exa 8.12 Calculating the equilibrium concentrations

```
1 # Page No. 198
2
3 library(polynom)
4
5 formula <- polynomial(c(0.011, -2.1, 99))
6 roots <- suppressWarnings(as.numeric(polyroot(
7   formula)))
8 Na_1 <- expression(0.110-10*x)
```

```
9 Cl_1 <- expression(0.100-10*x)
10 Na_2 <- expression(x)
11 Cl_2 <- expression(x)
12 print(eval({x <- roots;Na_1}))
13 print(eval({x <- roots;Cl_1}))
14 print(eval({x <- roots;Na_2}))
15 print(eval({x <- roots;Cl_2}))
16
17 # The answer provided in the textbook is wrong.
```

Chapter 9

Electrochemistry

R code Exa 9.1 Finding weight of copper plating on cathode and anode

```
1 # Page No. 209
2
3 I <- 0.500
4 t <- 55 * 60
5 F <- 96485.3
6 M <- 63.546
7
8 Q <- I * t
9 n <- Q / F
10 w <- n * (M / 2)
11
12 print(w)
```

R code Exa 9.2 Calculating transference numbers

```
1 # Page No. 211
2
3 m_1 <- 0.9972
```

```

4 m_2 <- 0.7532
5 m_cathode <- 0.4000
6 M <- 63.546
7
8 n_mig <- (m_1 / (M / 2)) - (m_2 / (M / 2))
9 n_mig2 <- -(n_mig - (m_cathode / (M / 2)))
10 t_neg <- n_mig / (m_cathode / (M / 2))
11 t_pos <- 1 - t_neg
12 t_neg2 <- n_mig2 / (m_cathode / (M / 2))
13 t_pos2 <- 1 - t_neg2
14
15 print(n_mig)
16 print(n_mig2)
17 print(t_neg)
18 print(t_pos)
19 print(t_neg2)
20 print(t_pos2)

```

R code Exa 9.3 Calculating equivalent conductance

```

1 # Page No. 217
2
3 K1 <- 0.002768
4 R1 <- 312
5 R2 <- 1043
6 c <- 0.01000
7
8 k <- K1 * R1
9 K2 <- k / R2
10 A <- K2 / (c / 1000)
11
12 print(k)
13 print(K2)
14 print(A)

```

R code Exa 9.4 Calculating equivalent conductance

```
1 # Page No. 218
2
3 lambda_H <- 349.8
4 lambda_Ac <- 40.9
5
6 ans <- sum(c(lambda_H, lambda_Ac))
7
8 print(ans)
```

R code Exa 9.5 Finding specific conductance

```
1 # Page No. 219
2
3 lambda_Ba <- 63.6
4 lambda_S04 <- 79.8
5 m <- 1 * 10^-3
6 M <- 233.38
7
8 lambda <- lambda_Ba + lambda_S04
9 c <- m / (M / 2)
10 K <- (c * lambda) / 1000
11
12 print(c)
13 print(K)
```

R code Exa 9.6 Finding E of cell

```
1 # Page No. 224
2
3 anode <- 0.763
4 cathode <- 0.337
5
6 E <- sum(c(anode, cathode))
7
8 print(E)
```

R code Exa 9.7 Calculating emf of the cell

```
1 # Page No. 227
2
3 a_Zn <- 1
4 a_Cu <- 1
5 a_Zn_pos <- 0.100
6 a_Cu_pos <- 0.0100
7 n <- 2
8 E <- 1.1
9 R <- 8.314
10 T <- 298
11 F <- 96485
12
13 Q <- (a_Cu * a_Zn_pos) / (a_Zn * a_Cu_pos)
14 E_cell <- E - (((R * T) / (n * F)) * log(Q))
15
16 print(E_cell)
```

R code Exa 9.8 Finding actual decomposition potential

```
1 # Page No. 233
2
3 V <- 1.23
```

```
4 V_Ag <- 0.15
5 V_0 <- 0.45
6
7 E <- sum(c(V, V_Ag, V_0))
8
9 print(E)
```

Chapter 10

Basic Quantum Mechanics

R code Exa 10.4 Finding coefficient h squared divided $2m$

```
1 # Page 248
2
3 h <- 6.626 * 10^-34
4 m <- 9.1094 * 10^-31
5 eV <- 1.60218 * 10^-19
6
7 k <- h^2 / (2 * m * eV)
8
9 print(k)
```

R code Exa 10.6 Calculating Fermi energy

```
1 # Page 253
2
3 d <- 10.50
4 A <- 6.022 * 10^23
5 m <- 107.9
6 h <- 6.626 * 10^-34
```

```

7 pi <- 3.141591
8 M_e <- 9.109 * 10^-31
9 e <- 1.6 * 10^-19
10
11 N <- (d * A * 10^6) / m
12 Ef <- {(h^2 / (8 * M_e)) * ((3 * N) / pi)^(2/3)} / e
13
14 print(N)
15 print(Ef)

```

R code Exa 10.7 Calculating coefficient h squared divided by 8m

```

1 # Page 258
2
3 h <- 6.626 * 10^-34
4 e <- 1.602 * 10^-19
5 m <- 9.10938 * 10^-31
6
7 c <- {h^2 / (8 * m)} / e
8
9 print(c)

```

R code Exa 10.8 Calculating kinetic energy

```

1 # Page 259
2
3 h <- 6.626 * 10^-34
4 e <- 1.602 * 10^-19
5 m <- 9.10938 * 10^-31
6 V <- 8
7
8 l <- 8^(1/3)
9 nx=ny=nz=1

```

```
10 a=b=c=1
11 k <- {{h^2 / (8 * m)} / e} * 10^20
12 E <- k * {(nx^2 / a^2) + (ny^2 / b^2) + (nz^2 / c^2)
    }
13
14 print(k)
15 print(E)
```

Chapter 11

Free Rotational and Angular Motion

R code Exa 11.4 Evaluating a constant h divided by 4π and c

```
1 # Page 282
2
3 h <- 1.05457 * 10^-27
4 pi <- 3.1415
5 c <- 2.99792 * 10^10
6
7 k <- h / (4 * pi * c)
8
9 print(k)
```

R code Exa 11.5 Calculating corresponding moment of inertia

```
1 # Page 282
2
3 h <- 1.05457 * 10^-27
4 pi <- 3.1415
```

```
5 c <- 2.99792 * 10^10
6 B <- 10.34
7
8 I <- h / (4 * pi * c * B)
9
10 print(I)
```

R code Exa 11.6 determining bond length in HCl

```
1 # Page 282
2
3 I <- 2.707 * 10^-40
4 m1 <- 1.00797
5 m2 <- 35.453
6 A <- 6.022 * 10^23
7
8 Mu <- (m1 * m2) / (m1 + m2)
9 Mu_grams <- Mu / A
10 r <- sqrt(I / Mu_grams)
11
12 print(r)
```

R code Exa 11.7 Expressing the Boltzmann constant in the reciprocal centimeter energy unit

```
1 # Page 289
2
3 h <- 6.626 * 10^-34
4 c <- 2.99792 * 10^10
5 Nu <- 2.08370057 * 10^10
6
7 k <- (h * Nu) / (h * c)
8
```

9 `print(k)`

Chapter 12

Vibrational and Radial Motion

R code Exa 12.6 Determining the force constant for a molecule

```
1 # Page 322
2
3 Mu <- 1.628 * 10^-24
4 pi <- 3.1415
5 c <- 2.9979 * 10^10
6 k <- 2990
7
8 f <- (Mu / 1000) * (2 * pi * c * k)^2
9
10 print(f)
11
12 # The answer may slightly vary due to rounding off
    values.
```

R code Exa 12.7 Calculating force constant of a spring

```
1 # Page 323
2
```

```
3 x <- 0.0100
4 m <- 0.100
5 g <- 9.81
6
7 f <- (m * g) / x
8
9 print(f)
```

R code Exa 12.9 Calculating the harmonic oscillator wave number

```
1 # Page 328
2
3 A <- matrix(c(1, 2, -2, -6), nrow= 2, ncol= 2)
4 B <- matrix(c(2886, 5668), nrow= 2, ncol= 1)
5
6 X <- solve(A,B)
7 rownames(X) <- c("1", "2")
8 a <- X[c(2)]
9 k <- X[c(1)]
10 b <- a / k
11
12 print(A)
13 print(B)
14 print(X)
15 print(k)
16 print(b)
```

R code Exa 12.10 Determining the dissociation energy of a diatomic molecule

```
1 # Page No. 328
2
3 k <- 2240
4 v <- 19.1
```

```
5
6 area <- (1/2) * k * v
7
8 print(area)
```

R code Exa 12.11 Evaluating Bohr radius

```
1 # Page 333
2
3 h <- 1.05457 * 10^-34
4 c <- 2.99792 * 10^8
5 Mu <- 9.10939 * 10^-31
6 e <- 1.60218 * 10^-19
7
8 k <- h^2 / (c^2 * Mu * 10^-7 * e^2)
9
10 cat(k, " / Z")
```

R code Exa 12.13 Expressing the electronic energy of a hydrogenlike system in reciprocal centimeters

```
1 # Page 333
2
3 h <- 6.62608 * 10^-34
4 b <- 2.17989 * 10^-18
5 c <- 2.99792 * 10^10
6
7 R <- b / (h * c)
8
9 print(R)
```

Chapter 13

Analyzing Organized Structures

R code Exa 13.16 Showing primitive symmetry species F2 occurs three times in the atomic motions

```
1 # Page 365
2
3 g <- 24
4 F2 <- c(3, 0, -1, -1, 1)
5 x <- c(15, 0, -1, -1, 3)
6 b <- c(1, 0, 3, 6, 6)
7
8 a <- (1/g) * sum(b * (F2 * x))
9
10 print(a)
```

Chapter 14

States of Molecular Electrons

R code Exa 14.3 estimating energies of molecular orbitals of HF

```
1 # Page 396
2
3 library(pracma)
4
5 I_1s <- 13.60
6 A_1s <- 0.75
7 I_2p <- 20.86
8 A_2p <- 3.50
9 B <- -2
10 n <- 1
11 pi <- 180
12
13 a_H <- -(I_1s + A_1s) / 2
14 a_F <- -(I_2p + A_2p) / 2
15 Zeta <- ((rad2deg(acot((a_H - a_F) / (2 * B)))) + (
    pi * n)) / 2
16 E1 <- a_F + (B * cot(deg2rad(Zeta)))
17 E2 <- a_H - (B * cot(deg2rad(Zeta)))
18 w1 <- sin((Zeta * 3.1415) / pi)
19 w2 <- cos((Zeta * 3.1415) / pi)
20 W1 <- paste("(", w2, "* w_H)", "+ (" , w1, "* w_F)")
```



```
21 W2 <- paste("(" , w1 , "*" w_H)" , "-" ( , w2 , "*" w_F)")
22
23 print(Zeta)
24 print(E1)
25 print(E2)
26 print(W1)
27 print(W2)
28
29 # The answer may slightly vary due to rounding off
    values.
```

Chapter 15

Phenomenological Chemical Kinetics

R code Exa 15.3 Estimating the order of the reaction

```
1 # Page 413
2
3 p_1 <- 7.49
4 p_2 <- 5.14
5 a <- 100
6 x_1 <- 5
7 x_2 <- 20
8
9 n <- (log(p_1) - log(p_2)) / (log(a - x_1) - log(a -
      x_2))
10
11 print(n)
```

R code Exa 15.4 Calculating the reaction order

```
1 # Page 415
```

```

2
3 t_1 <- 410
4 t_2 <- 880
5 p_1 <- 363
6 p_2 <- 169
7
8 n <- ((log(t_2) - log(t_1)) / (log(p_1) - log(p_2)))
      + 1
9
10 print(n)

```

R code Exa 15.7 Calculating the Arrhenius parameters

```

1 # Page 417
2
3 k_1 <- 8.90 * 10^-5
4 T_1 <- 283 + 273.15
5 k_2 <- 5.04 * 10^-3
6 T_2 <- 356 + 273.15
7 R <- 8.3145
8
9 E_a <- (R * T_2 * T_1 * log(k_2 / k_1)) / (T_2 - T_
      1)
10 A <- exp(log(k_1) + (E_a / (R * T_1)))
11
12 print(E_a)
13 print(A)

```

R code Exa 15.8 Calculating the rate constants

```

1 # Page 420
2
3 K <- 1.002 * 10^-14

```

```

4 t <- 37 * 10^-6
5 m <- 1000
6 M <- 18.015
7
8 b <- c <- sqrt(K)
9 C <- m / M
10 K_c <- K / C
11 k_1 <- 1 / (t * (K_c + b + c))
12 k <- k_1 * K_c
13
14 print(k)

```

R code Exa 15.9 Calculating the diffusion limited rate constant

```

1 # Page 426
2
3 R <- 8.3145
4 T <- 25 + 273.15
5 n <- 0.891 * 10^-3
6
7 k <- (8 * R * T * 10^3) / (3 * n)
8
9 print(k)

```

R code Exa 15.10 Calculating the zero activation energy rate constant

```

1 # Page 426
2
3 R <- 8.3145
4 T <- 25 + 273.15
5 pi <- 3.14159
6 r_a <- r_b <- 2.2 * 10^-10
7 M <- 15 * 10^-3

```

```
8 N <- 6.0221 * 10^23
9 k <- 7.42 * 10^9
10
11 sigma <- pi * (2 * r_a)^2
12 vel <- sqrt((16 * R * T) / (pi * M))
13 k_AB <- sigma * vel * N * 10^3
14 ratio <- k_AB / k
15
16 print(k_AB)
17 print(ratio)
```

Chapter 16

Explanatory Mechanisms

R code Exa 16.2 Calculating coefficient k

```
1 # Page 453
2
3 y_S205 <- 0.661
4 y_I <- 0.899
5 y <- 0.405
6 k_1 <- 1.33
7 y_S205_2 <- 0.804
8 y_I_2 <- 0.946
9 y_2 <- 0.616
10
11 K_o <- (k_1 * y) / (y_S205 * y_I)
12 K <- K_o * (y_S205_2 * y_I_2) / y_2
13
14 print(K)
```

Chapter 17

Statistical Thermodynamics

R code Exa 17.12 Formulating K_c and K_p

```
1 # Page No. 472
2
3 e <- 2.71828
4 D <- 70.4 * 10^3
5 R <- 8.31451
6 T <- 1000
7 n <- 1
8
9 z_el <- 1
10 z_rot <- 2.24641 * T
11 z_vib <- 1 / (1 - e^-(229.05 / T))
12 z_tr <- (5.8594 * 10^28) * T^1.5
13 f <- (-D / (R * T))
14
15 z_Na2 <- z_el * z_rot * z_vib * z_tr
16 z_Na <- (4.1432 * 10^28) * T^1.5
17 K_c <- ((z_Na^2 / z_Na2) * e^-(D / (R * T))) /
      (6.0221 * 10^26)
18
19 K_p <- K_c * (R / 100 * T)^n
20
```

```
21 print(K_c)
22 print(K_p)
```

R code Exa 17.13 Calculating the constant products

```
1 # Page 476
2
3 h <- 6.626 * 10^-34
4 c <- 2.99792 * 10^8
5 k <- 1.38066 * 10^-23
6 pi <- 3.1415
7
8 k_1 <- (8 * h * c * pi)
9 k_2 <- (h * c) / k
10
11 print(k_1)
12 print(k_2)
```

R code Exa 17.14 Calculating electromagnetic energy

```
1 # Page 477
2
3 h <- 6.626 * 10^-34
4 c <- 2.99792 * 10^8
5 k <- 1.38066 * 10^-23
6 pi <- 3.1415
7 lambda <- 512.5 * 10^-9
8 e <- 2.7182
9 T <- 2000
10 lambda_change <- 25 * 10^-9
11 v <- 1 * 10^-6
12
13 k_1 <- (8 * h * c * pi) / lambda^5
```



```
14 k_2 <- e^((h * c) / (lambda * k * T))
15 Rho <- k_1 * (1 / (k_2 - 1))
16 E <- Rho * lambda_change * v
17
18 print(Rho)
19 print(E)
```

R code Exa 17.15 Evaluating coefficient of integral in formula

```
1 # Page 482
2
3 h <- 6.626 * 10^-34
4 pi <- 3.1415
5 m <- 9.1094 * 10^-31
6
7 c <- (4 * pi * (2 * m)^1.5) / h^3
8
9 print(c)
```

Chapter 18

Reaction Rate Theory

R code Exa 18.6 Estimating the maximum kinetic isotope effect

```
1 # Page 493
2
3 k1 <- 3300
4 Mu1 <- 1.007825
5 Mu2 <- 2.0140
6 e <- 2.71828
7 k <- 0.69504
8 T <- 298.15
9
10 lambda <- (1/2) * k1 * (1 - sqrt(Mu1 / Mu2))
11 k2_k1 <- exp(-lambda / (k * T))
12 k1_k2 <- 1 / k2_k1
13
14 print(k2_k1)
15 print(k1_k2)
```

R code Exa 18.8 Calculating the thermodynamic properties M and S and G

```
1 # Page 503
2
3 k <- 1.76 * 10^13
4 h <- 6.62608 * 10^-34
5 kb <- 1.38066 * 10^-23
6 T <- 202.50
7 e <- 2.71828
8 R <- 8.31451
9 E_a <- 46860
10
11 k_1 <- (e * ((kb * T) / h))
12 K <- k / k_1
13 S <- R * log (K)
14 H <- E_a - (R * T)
15 G <- H - (T * S)
16
17 print(S)
18 print(H)
19 print(G)
20
21 # The answer may slightly vary due to rounding off
    values.
```

Chapter 19

Photochemistry

R code Exa 19.1 Calculating the transmittance at the same wavelength of two filters in combination

```
1 # Page 510
2
3 I1_I0 <- 0.727
4 I2_I1 <- 0.407
5
6 I2_I0 <- I1_I0 * I2_I1
7
8 print(I2_I0)
```

R code Exa 19.3 Calculating the photon energy

```
1 # Page 512
2
3 e <- 1.6 * 10^-19
4 E_photon <- 1 * 10^-3
5 c <- 2.99792 * 10^8
6 M <- 5.6857 * 10^-12
```

```
7
8 k <- 2 * M * c^2
9 E <- k * E_photon * e
10
11 print(E)
```

R code Exa 19.4 Calculating the absorbance A and the molar absorption coefficient E

```
1 # Page 514
2
3 I_I0 <- 0.160
4 l <- 0.100
5 B <- 0.0500
6
7 A <- -log10(I_I0)
8 E <- A / (B * l)
9
10 print(A)
11 print(E)
```

R code Exa 19.5 Evaluate the product $N \times h \times c$

```
1 # Page 514
2
3 h <- 6.62608 * 10^-34
4 c <- 2.99792 * 10^8
5 N <- 6.022 * 10^23
6
7 k <- N * h * c
8
9 print(k)
```

R code Exa 19.6 Calculating oscillator strength

```
1 # Page 515
2
3 k <- 1.0645
4 k_1 <- 4.32 * 10^-9
5 e_max <- 44000
6 v <- 5000
7
8 K <- k * e_max * v
9 f <- K * k_1
10
11 print(K)
12 print(f)
```
