R Textbook Companion for
Modern Physical Chemistry: A Molecular Approach
by George H. Duffey[1]

Created by
Ojas Singh
12th (Senior Secondary)
PCMB (Physics, Chemistry, Mathematics & Biology)
Apeejay School, Noida
Cross-Checked by
R TBC Team

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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

```
# Page No. 3

n <- 1
lambda <- 0.70*10^-8
d <- 1/200
mins <- 5
mins_deg <- 60
radian <- 3.1416

theta <- (mins*radian)/(mins_deg*180)
phi <- sqrt(((n * lambda * 2) / d) + theta^2)

print(theta)
print(phi)
```

R code Exa 1.2 Finding interplanar spacing

```
# Page No. 6
```

```

library(pracma)

n <- 1
lambda <- 1.539
theta <- deg2rad(37.25)

d <- lambda  / (2 * sin(theta))

print(d)
```

R code Exa 1.6 Calculating Avogadros number

```
# Page No. 17

n <- 4
rho <- 2.640
V <- 4.016*10^-8
M <- 25.939

m <- (rho * (V)^3) /  n
N_a <- M / m

print(m)
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

```
# Page No. 26

h <- 6.6261*10^-34
m <- 9.1094*10^-31
e <- 1.6022*10^-19

lambda <- h/sqrt(2*m*e)

print(lambda)
cat(lambda,”/V^(1/2)”,sep = ””)
```

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

```
# Page No. 32
```

```r

x <- 0.083
A <- 6.02*10^23
m <- 8.642
M <- 112.41
I <- 1*10^-4

n <- (m / M) * A
sigma <- -log(I) / (n * x)

print(n)
print(sigma)
```

Chapter 3

Gases and Collective Properties

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

```
# Page No. 40

g <- 9.80665
h <- 0.7600
m <- 13595.1

P <- g * h * m

print(P)
```

R code Exa 3.3 Calculating joules in 1 liter atmosphere

```
# Page No. 40

P <- 101325
v <- 10^3
Mu <- 10^-2

```

```
V <- v * (Mu^3)
J <- P * V

print(V)
print(J)
```

R code Exa 3.4 Changing the energy unit in R

```
# Page No. 43

r <- 8.31451
c <- 0.1
cal <- 4.18400

R <- r / c
R_1 <- r / cal

print(R)
print(R_1)
```

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

```
# Page No. 43

R <- 8.31451
T <- 293.15
M <- 0.0040026

u <- sqrt((3 * R * T) / M)

print(u)
```

R code Exa 3.6 Calculating the partial pressure

```
# Page No. 44

n <- 15
P <- 720
n_1 <- 2
n_2 <- 10
n_3 <- 3

P_N2 <- (n_1 / n) * P
P_O2 <- (n_2 / n) * P
P_CO2 <- (n_3 / n) * P

print(P_N2)
print(P_O2)
print(P_CO2)
```

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

```
# Page No. 46

n <- 1
R <- 8.31451
T <- 298.151
E_vib <- 0
E_el <- 0

E_tr <- 1.5 * n * R * T
E_rot <- 1.5 * n * R * T
E <- E_tr + E_rot + E_vib + E_el
```

```

print(E_tr)
print(E_rot)
print(E)

# The answer may slightly vary due to rounding off
   values.
```

R code Exa 3.8 Calculating radius of helium atom

```
# Page No. 48

b <- 24.1
pi <- 3.1416
N <- 6.022 * 10^23

r <- ((3 * b)/(16 * pi * N))^(1/3)

print(r)
```

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

```
# Page No. 54

pi <- 3.1416
r <- 4.5 * 10^-7
p <- 18.3
g <- 9.807
d <- 1000
h <- 0.200 * 10^-2
N_0 <- 89
k <- 1.3807 * 10^-23
T <- 298.15
```

```

V <- (4/3) * pi * (r^3)
F <- (p / d) * g * V
E <- F * h
N_1 <- exp(-E / (k * T))
N <- N_1 * N_0

print(V)
print(F)
print(E)
print(N_1)
print(N)

# 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

```
# Page No. 59

pi <- 3.1416
r <- 3.61 * 10^-10
R <- 8.31451
T <- 298.15
M <- 31.999 * 10^-3
k <- 1.3807 * 10^-23
P <- 1 * 10^5

alpha <- pi * (r^2)
v <- sqrt((16 * R * T) / (pi * M))
d <- P / (k * T)
Z <- 0.5 * alpha * v * (d^2)

print(alpha)
```

```
print(v)
print(d)
print(Z)
```

R code Exa 3.14 Calculating hypothetical maximum specific reaction rate

```
# Page No. 59

a <- 4.094 * 10^-19
v <- 628.1337
N_a <- 6.022 * 10^23

k_aa <- 0.5 * a * v * N_a * 1000

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

```
# Page No. 69

h <- 40893
mol <- 1
R <- 8.31451
T <- 372.778

q <- mol * h
w <- -R * T
E <- q + w
H <- q

print(E)
print(H)
```

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

```r
# Page No. 72

w <- 0
E <- 0

q <- E - w

print(q)
```

R code Exa 4.6 Estimating translational and rotational and vibrational contributions

```r
# Page No. 75

R <- 8.31451
Cv_500 <- 26.90

Cv_tr <- 3  * R / 2
Cv_rot <- 3 * R /2
Cv_vib <- Cv_500 - (Cv_tr + Cv_rot)

print(Cv_rot)
print(Cv_tr)
print(Cv_vib)
```

Chapter 5

Entropy and the Second Law

R code Exa 5.1 Calculating entropy change

```
# Page No. 89

q <- 1590
C <- 32.1

T <- C + 273
S <- q / T

print(S)
```

R code Exa 5.2 Calculating entropy change

```
# Page No. 89

n <- 1
R <- 8.31451
T1 <- 323.15
T2 <- 373.15
```

```

S <- 2.5 * n * R * log(T2/T1)

print(S)
```

R code Exa 5.4 Calculating entropy change

```
# Page No. 93

w <- 0.001
k <- 1.3807 * 10^-23

S <- k * log(w)

print(S)
```

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

```
# Page No. 96

w <- -3099

A <- q + w - q
G <- q - q

print(A)
print(G)
```

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

```
# Page No. 101

x <- 10
c <- log(2)
R <- 8.31451
T <- 298.15

a <- c / x
F <- (R * T * c * 100) / x

print(F)
```

R code Exa 5.9 Determining the gravitational force

```
# Page No. 102

M <- 0.100
g <- 9.807

F <- -M  * g

print(F)
```

Chapter 6

Relationships between Phases

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

```r
# Page No. 112

n <- 2
R <- 8.31451
C <- 40
X_a <- 0.5
X_b <- 0.5

T <- C + 273.15
q <- -n * R * T * (X_a * log(X_a) + X_b * log(X_b))

print(q)

# The answer may slightly vary due to rounding off
   values.
```

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

```
# Page No. 122

T1 <- 273.15
V <- -0.0906
L <- 333.5
j <- 0.101325
P1 <- 760
P2 <- 4.6

P <- ((P2 - P1) / P1) * j
T <- (T1 * V * P) / L

print(P)
print(T)
```

R code Exa 6.4 Calculating the vapour pressure of benzene

```
# Page No. 124

T <- 333.15
C <- 17.6254
slope <- 3884

P <- exp((-slope / T) + C)

print(P)
```

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

```
# Page No. 125

R <- 0.08206
T <- 298.15
```

```
P_A <- 23.8
V <- 0.018
pp <- 6
P_a <- 760

P_1 <- pp - (P_A / P_a)
P <- (V * P_A * P_1) / (R * T)
final_P <- P + P_A

print(P_1)
print(P)
print(final_P)
```

R code Exa 6.6 Finding initial concentration of methanol in vaporu

```
# Page No. 127

X_A <- 0.250
X_B <- 0.750
VP_CH3OH <- 96
VP_C2H5OH <- 43.9

PCH3OH <- X_A * VP_CH3OH
PC2H5OH <- X_B * VP_C2H5OH
P <- PC2H5OH + PCH3OH
X_CH3OH <- PCH3OH / P

print(PC2H5OH)
print(PCH3OH)
print(X_CH3OH)
```

R code Exa 6.7 Calculating the molal elevation constant for water

```r
# Page No. 130

R <- 8.31451
T <- 372.78
L <- 40671
M <- 18.015

K_b <- (R * (T^2) * M) / (L * 1000)

print(K_b)
```

R code Exa 6.8 Calculating osmotic pressure for a sucrose solution

```r
# Page No. 135

M <- 0.100
C <- 30
R <- 0.08206

T <- C + 273.15
w <- 1000 / M
V <- w / 1000
P <- (R * T) / V

print(P)
```

Chapter 7

Relationships among Reactants

R code Exa 7.2 Determining delta H for a reaction

```
# Page No. 144

H_eqn1 <- -241.83
H_eqn2 <- -136.11

H_eqn <- (2 * -H_eqn1) + H_eqn2

print(H_eqn)
```

R code Exa 7.5 Calculating entropy correction for gas imperfection

```
# Page No. 150

R <- 8.31451
P <- 1.000
P_c <- 33.9
T_c <- 126
T <- 77.32
```

```

S <- (27 / 32) * R * (P / P_c) * ((T_c / T)^3)

print(S)
```

R code Exa 7.6 Calculating delta S and G and H

```
# Page No. 151

S_NO2 <- 240.02
S_NO <- 210.76
S_O2 <- 205.15
H_NO2 <- 33.10
H_NO <- 90.29
H_O2 <- 0
G_NO2 <- 51.26
G_NO <- 86.60
G_O2 <- 0

S <- S_NO2 - S_NO - (0.5 * S_O2)
H <- H_NO2 - H_NO - (0.5 * H_O2)
G <- G_NO2 - G_NO - (0.5 * H_O2)

print(S)
print(G)
print(H)
```

R code Exa 7.7 Calculating Gibbs energy change

```
# Page No. 155

P_H2O <- 0.0500
P_H2 <- 0.0100
```

```
P_O2 <- 0.1000
G_o <- -228.62
R <- 8.31451
T <- 298.15


Q <- P_H2O / (P_H2 * sqrt(P_O2))
G <- G_o + (R * 10^-3 * T * log(Q))

print(Q)
print(G)
```

R code Exa 7.8 Determining the equilibrium constant

```
# Page No. 156

Kf_H2O <- 40.053
Kf_H2 <- 0
Kf_O2 <- 0

log_K <- (Kf_H2O) - Kf_H2 - (0.5 * Kf_O2)
K <- 10^log_K

print(log_K)
print(K)
```

R code Exa 7.9 Calculating Kp and Kc

```
# Page No. 159

R <- 0.083145
C <- 25
K_p <- 1.130 * 10^40
```

```
n <- -1/2

T <- C + 273.15
K <- K_p * (R * T)^-n

print(K)
```

R code Exa 7.11 Calculating Kp

```
# Page No. 160

K_N2O4 <- -17.132
K_NO2 <- -8.981

K <- 10^((2 * (K_NO2)) - (K_N2O4))

print(K)
```

R code Exa 7.12 Calculating the density of an equilibrium mixture

```
# Page No. 160

w <- 0.148
P <- 1
M <- 92.011
R <- 0.083145
T <- 298.15
v <- 2

a <- sqrt(w / (4 + w))
rho <- (P * M) / (R * T * (1 + ((v - 1) * a)))

print(a)
```

```
print(rho)
```

R code Exa 7.13 Calculating final pressure after equilibrium

```
# Page 161

library(polynom)

kp <- 0.0562
ml <- 0.5

x <- solve(polynomial(c(-kp,0.5,1)))[solve(polynomial(c(-kp,0.5,1)))>0]

print(x+kp/x)
```

Chapter 8

Equilibria in Condensed Phases

R code Exa 8.1 Calculating amount of I2 in equilibrium

```
# Page No. 174

library(Ryacas)

mol <- 0.0200
MF <- 812
n <- yac_symbol("n")

x <- eval(yac_expr(simplify(mol / (((MF * n) / n) +
   2))))

print(x)
```

R code Exa 8.2 Calculating hydrogen ion concentration in a solution

```
# Page No. 175

K <- 1.749 * 10^-5
```

```
C_CH3COOH <- 0.100
C_CH3COO <- 0.0100

C_H <- (C_CH3COOH / C_CH3COO) * K

print(C_H)
```

R code Exa 8.3 Calculating hydrogen ion concentration

```
# Page No. 175

library(polynom)

Kc <- 1.749 * 10^-5
M <- 0.0100

k <- M * Kc
x <- solve(polynomial(c(-k,Kc,1)))[solve(polynomial(
   c(-k,Kc,1))>0]

print(x)
```

R code Exa 8.4 Calculate the hydroxide ion concentration

```
# Page No. 176

K <- 1.749 * 10^-5
K_m <- 1.008 * 10^-14
m_CH3COOH <- x
m_CH3COO <- 0.100

x <- sqrt((m_CH3COO * K_m) / K)

```

```
print(x)
```

R code Exa 8.5 Calculating mH

```
# Page No. 179

m_1 <- 7.47 * 10^-5
m_2 <- 4.57 * 10^-3
mH_mOH <- 1.008 * 10^-14

MH_MOH <- m_2 / m_1
mH <- sqrt(mH_mOH * MH_MOH)

print(mH)
```

R code Exa 8.6 Calculating mH

```
# Page No. 180

m_1 <- 1.75 * 10^-5
m_2 <- 1.772 * 10^-4
mH_mOH <- 1.008 * 10^-14

MH_MOH <- m_2 / m_1
mH <- sqrt(mH_mOH * MH_MOH)

print(mH)
```

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

```
# Page No. 183

S_H <- 0
S_HCOO <- 92
S_HCOOH <- 163
H_H <- 0
H_HCOO <- -425.55
H_HCOOH <- -425.43
logKf_H <- 0
logKf_HCOO <- 61.49
logKf_HCOOH <- -65.22

S <- S_H + S_HCOO - S_HCOOH
H <- H_H + H_HCOO - H_HCOOH
K <- 10^(logKf_H + logKf_HCOO + logKf_HCOOH)

print(S)
print(H)
print(K)

# The answer provided in the textbook is wrong.
```

R code Exa 8.9 Calculating hydrogen ion concentration

```
# Page No. 191

library(polynom)

K <- 1.754 * 10^-5
Y_HA <- 1
m_Na <- 0.100
z_Na <- 1
m_Cl <- 0.100
z_Cl <- 1
Y_H <- 0.825
```

```
Y_A <- 0.775
K_1 <- 2.743 * 10^-6

k <- (Y_HA / (Y_A * Y_H)) * K
x <- solve(polynomial(c(-K_1,k,1)))[solve(polynomial
   (c(-K_1,k,1)))>0]

print(x)
```

R code Exa 8.10 Calculating hydrogen ion concentration

```
# Page No. 194

library(polynom)

K <- 1.754 * 10^-5
Y_HA <- 1
Y_H <- 1
Y_A <- 1

K_3 <- (Y_HA / (Y_H * Y_A)) * K
x <- solve(polynomial(c(-K_3 / 10,K_3,1)))[solve(
   polynomial(c((-K_3 / 10),K_3,1)))>0]

Y2_H <- 0.963
Y2_A <- 0.961

k <- (Y_HA / (Y2_A * Y2_H)) * K
X <- solve(polynomial(c(-k / 10,k,1)))[solve(
   polynomial(c((-k / 10),k,1)))>0]

print(K_3)
print(x)
print(k)
print(X)
```

R code Exa 8.11 Calculating the solubility of AgCI

```
# Page No. 195

library(polynom)

K <- 1.768 * 10^-10
Y_Cl <- 0.755
Y_Ag <- 0.745
MM <- 143.321

K_1 <- (1 / (Y_Cl * Y_Ag)) * K
x <- sqrt(K_1)
w <- x * MM

print(x)
print(w)

# The answer provided in the textbook is wrong.
```

R code Exa 8.12 Calculating the equilibrium concentrations

```
# Page No. 198

library(polynom)

formula <- polynomial(c(0.011,-2.1,99))
roots <- suppressWarnings(as.numeric(polyroot(
   formula)))
roots <- roots[1]
Na_1 <- expression(0.110-10*x)
```

```
Cl_1 <- expression(0.100-10*x)
Na_2 <- expression(x)
Cl_2 <- expression(x)
print(eval({x <- roots;Na_1}))
print(eval({x <- roots;Cl_1}))
print(eval({x <- roots;Na_2}))
print(eval({x <- roots;Cl_2}))

# 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

```
# Page No. 209

I <- 0.500
t <- 55 * 60
F <- 96485.3
M <- 63.546

Q <- I * t
n <- Q / F
w <- n * (M / 2)

print(w)
```

R code Exa 9.2 Calculating transference numbers

```
# Page No. 211

m_1 <- 0.9972
```

```
m_2 <- 0.7532
m_cathode <- 0.4000
M <- 63.546

n_mig <- (m_1 / (M / 2)) - (m_2 / (M / 2))
n_mig2 <- -(n_mig - (m_cathode / (M / 2)))
t_neg <- n_mig / (m_cathode / (M / 2))
t_pos <- 1 - t_neg
t_neg2 <- n_mig2 / (m_cathode / (M / 2))
t_pos2 <- 1 - t_neg2

print(n_mig)
print(n_mig2)
print(t_neg)
print(t_pos)
print(t_neg2)
print(t_pos2)
```

R code Exa 9.3 Calculating equivalent conductance

```
# Page No. 217

K1 <- 0.002768
R1 <- 312
R2 <- 1043
c <- 0.01000

k <- K1 * R1
K2 <- k / R2
A <- K2 / (c / 1000)

print(k)
print(K2)
print(A)
```

R code Exa 9.4 Calculating equivalent conductance

```
# Page No. 218

lambda_H <- 349.8
lambda_Ac <- 40.9

ans <- sum(c(lambda_H, lambda_Ac))

print(ans)
```

R code Exa 9.5 Finding specific conductance

```
# Page No. 219

lambda_Ba <- 63.6
lambda_SO4 <- 79.8
m <- 1 * 10^-3
M <- 233.38

lambda <- lambda_Ba + lambda_SO4
c <- m / (M / 2)
K <- (c * lambda) / 1000

print(c)
print(K)
```

R code Exa 9.6 Finding E of cell

```r
# Page No. 224

anode <- 0.763
cathode <- 0.337

E <- sum(c(anode, cathode))

print(E)
```

R code Exa 9.7 Calculating emf of the cell

```r
# Page No. 227

a_Zn <- 1
a_Cu <- 1
a_Zn_pos <- 0.100
a_Cu_pos <- 0.0100
n <- 2
E <- 1.1
R <- 8.314
T <- 298
F <- 96485

Q <- (a_Cu * a_Zn_pos) / (a_Zn * a_Cu_pos)
E_cell <- E - (((R * T) / (n * F)) * log(Q))

print(E_cell)
```

R code Exa 9.8 Finding actual decomposition potential

```r
# Page No. 233

V <- 1.23
```

```r
V_Ag <- 0.15
V_O <- 0.45

E <- sum(c(V, V_Ag, V_O))

print(E)
```

Chapter 10

Basic Quantum Mechanics

R code Exa 10.4 Finding coefficient h squared divided 2m

```r
# Page 248

h <- 6.626 * 10^-34
m <- 9.1094 * 10^-31
eV <- 1.60218 * 10^-19

k <- h^2 / (2 * m * eV)

print(k)
```

R code Exa 10.6 Calculating Fermi energy

```r
# Page 253

d <- 10.50
A <- 6.022 * 10^23
m <- 107.9
h <- 6.626 * 10^-34
```

```
pi <- 3.141591
M_e <- 9.109 * 10^-31
e <- 1.6 * 10^-19

N <- (d * A * 10^6) / m
Ef <- {(h^2 / (8 * M_e)) * ((3 * N) / pi)^(2/3)} / e

print(N)
print(Ef)
```

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

```
# Page 258

h <- 6.626 * 10^-34
e <- 1.602 * 10^-19
m <- 9.10938 * 10^-31

c <- {h^2 / (8 * m)} / e

print(c)
```

R code Exa 10.8 Calculating kinetic energy

```
# Page 259

h <- 6.626 * 10^-34
e <- 1.602 * 10^-19
m <- 9.10938 * 10^-31
V <- 8

l <- 8^(1/3)
nx=ny=nz=1
```

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

print(k)
print(E)
```

Chapter 11

Free Rotational and Angular Motion

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

```r
# Page 282

h <- 1.05457 * 10^-27
pi <- 3.1415
c <- 2.99792 * 10^10

k <- h / (4 * pi * c)

print(k)
```

R code Exa 11.5 Calculating corresponding moment of inertia

```r
# Page 282

h <- 1.05457 * 10^-27
pi <- 3.1415
```

```r
c <- 2.99792 * 10^10
B <- 10.34

I <- h / (4 * pi * c * B)

print(I)
```

R code Exa 11.6 determining bond length in HCl

```r
# Page 282

I <- 2.707 * 10^-40
m1 <- 1.00797
m2 <- 35.453
A <- 6.022 * 10^23

Mu <- (m1 * m2) / (m1 + m2)
Mu_grams <- Mu / A
r <- sqrt(I / Mu_grams)

print(r)
```

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

```r
# Page 289

h <- 6.626 * 10^-34
c <- 2.99792 * 10^10
Nu <- 2.08370057 * 10^10

k <- (h * Nu) / (h * c)

```

```
print(k)
```

Chapter 12

Vibrational and Radial Motion

R code Exa 12.6 Determining the force constant for a molecule

```
# Page 322

Mu <- 1.628 * 10^-24
pi <- 3.1415
c <- 2.9979 * 10^10
k <- 2990

f <- (Mu / 1000) * (2 * pi * c * k)^2

print(f)

# The answer may slightly vary due to rounding off
   values.
```

R code Exa 12.7 Calculating force constant of a spring

```
# Page 323

```

```
x <- 0.0100
m <- 0.100
g <- 9.81

f <- (m * g) / x

print(f)
```

R code Exa 12.9 Calculating the harmonic oscillator wave number

```
# Page 328

A <- matrix(c(1, 2, -2, -6), nrow= 2, ncol= 2)
B <- matrix(c(2886, 5668), nrow= 2, ncol= 1)

X <- solve(A,B)
rownames(X) <- c("1","2")
a <- X[c(2)]
k <- X[c(1)]
b <- a / k

print(A)
print(B)
print(X)
print(k)
print(b)
```

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

```
# Page No. 328

k <- 2240
v <- 19.1
```

```r

area <- (1/2) * k * v

print(area)
```

R code Exa 12.11 Evaluating Bohr radius

```r
# Page 333

h <- 1.05457 * 10^-34
c <- 2.99792 * 10^8
Mu <- 9.10939 * 10^-31
e <- 1.60218 * 10^-19

k <- h^2 / (c^2 * Mu * 10^-7 * e^2)

cat(k, ”/ Z”)
```

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

```r
# Page 333

h <- 6.62608 * 10^-34
b <- 2.17989 * 10^-18
c <- 2.99792 * 10^10

R <- b / (h * c)

print(R)
```

Chapter 13

Analyzing Organized Structures

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

```
# Page 365

g <- 24
F2 <- c(3, 0, -1, -1, 1)
x <- c(15, 0, -1, -1, 3)
b <- c(1, 0, 3, 6, 6)

a <- (1/g) * sum(b * (F2 * x))

print(a)
```

Chapter 14

States of Molecular Electrons

R code Exa 14.3 estimating energies of molecular orbitals of HF

```
# Page 396

library(pracma)

I_1s <- 13.60
A_1s <- 0.75
I_2p <- 20.86
A_2p <- 3.50
B <- -2
n <- 1
pi <- 180

a_H <- -(I_1s + A_1s) / 2
a_F <- -(I_2p + A_2p) / 2
Zeta <- ((rad2deg(acot((a_H - a_F) / (2 * B)))) + (
   pi * n)) / 2
E1 <- a_F + (B * cot(deg2rad(Zeta)))
E2 <- a_H - (B * cot(deg2rad(Zeta)))
w1 <- sin((Zeta * 3.1415) / pi)
w2 <- cos((Zeta * 3.1415) / pi)
W1 <- paste(”(”, w2, ”* w_H)” ,”+ (”, w1, ”* w_F)”)
```

```
W2 <- paste(”(”, w1, ”* w_H)” ,”– (”, w2, ”* w_F)”)

print(Zeta)
print(E1)
print(E2)
print(W1)
print(W2)

# 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

```r
# Page 413

p_1 <- 7.49
p_2 <- 5.14
a <- 100
x_1 <- 5
x_2 <- 20

n <- (log(p_1) - log(p_2)) / (log(a - x_1) - log(a - x_2))

print(n)
```

R code Exa 15.4 Calculating the reaction order

```r
# Page 415
```

```r

t_1 <- 410
t_2 <- 880
p_1 <- 363
p_2 <- 169

n <- ((log(t_2) - log(t_1)) / (log(p_1) - log(p_2)))
    + 1

print(n)
```

R code Exa 15.7 Calculating the Arrhenius parameters

```r
# Page 417

k_1 <- 8.90 * 10^-5
T_1 <- 283 + 273.15
k_2 <- 5.04 * 10^-3
T_2 <- 356 + 273.15
R <- 8.3145

E_a <- (R * T_2 * T_1 * log(k_2 / k_1)) / ( T_2 - T_
    1)
A <- exp(log(k_1) + (E_a / (R * T_1)))

print(E_a)
print(A)
```

R code Exa 15.8 Calculating the rate constants

```r
# Page 420

K <-  1.002 * 10^-14
```

```r
t <- 37 * 10^-6
m <- 1000
M <- 18.015

b <- c <- sqrt(K)
C <- m / M
K_c <- K / C
k_1 <- 1 / (t * (K_c + b + c))
k <- k_1 * K_c

print(k)
```

R code Exa 15.9 Calculating the diffusion limited rate constant

```r
# Page 426

R <- 8.3145
T <- 25 + 273.15
n <- 0.891 * 10^-3

k <- (8 * R * T * 10^3) / (3 * n)

print(k)
```

R code Exa 15.10 Calculating the zero activation energy rate constant

```r
# Page 426

R <- 8.3145
T <- 25 + 273.15
pi <- 3.14159
r_a <- r_b <- 2.2 * 10^-10
M <- 15 * 10^-3
```

```
N <- 6.0221 * 10^23
k <- 7.42 * 10^9

sigma <- pi * (2 * r_a)^2
vel <- sqrt((16 * R * T) / (pi * M))
k_AB <- sigma * vel * N * 10^3
ratio <- k_AB / k

print(k_AB)
print(ratio)
```

Chapter 16

Explanatory Mechanisms

R code Exa 16.2 Calculating coefficient k

```
# Page 453

y_S205 <- 0.661
y_I <- 0.899
y <- 0.405
k_1 <- 1.33
y_S205_2 <- 0.804
y_I_2 <- 0.946
y_2 <- 0.616

K_o <- (k_1 * y) / (y_S205 * y_I)
K <- K_o * (y_S205_2 * y_I_2) / y_2

print(K)
```

Chapter 17

Statistical Thermodynamics

R code Exa 17.12 Formulating Kc and Kp

```
# Page No. 472

e <- 2.71828
D <- 70.4 * 10^3
R <- 8.31451
T <- 1000
n <- 1

z_el <- 1
z_rot <- 2.24641 * T
z_vib <-  1 / (1 - e^-(229.05 / T))
z_tr <- (5.8594 * 10^28) * T^1.5
f <- (-D / (R * T))

z_Na2 <- z_el * z_rot * z_vib * z_tr
z_Na <- (4.1432 * 10^28) * T^1.5
K_c <- ((z_Na^2 / z_Na2) * e^-(D / (R * T))) /
   (6.0221 * 10^26)

K_p <- K_c * (R / 100 * T)^n

```

```
print(K_c)
print(K_p)
```

R code Exa 17.13 Calculating the constant products

```
# Page 476

h <- 6.626 * 10^-34
c <- 2.99792 * 10^8
k <- 1.38066 * 10^-23
pi <- 3.1415

k_1 <- (8 * h * c * pi)
k_2 <- (h * c) / k

print(k_1)
print(k_2)
```

R code Exa 17.14 Calculating electromagnetic energy

```
# Page 477

h <- 6.626 * 10^-34
c <- 2.99792 * 10^8
k <- 1.38066 * 10^-23
pi <- 3.1415
lambda <- 512.5 * 10^-9
e <- 2.7182
T <- 2000
lambda_change <- 25 * 10^-9
v <- 1 * 10^-6

k_1 <- (8 * h * c * pi) / lambda^5
```

```r
k_2 <- e^((h * c) / (lambda * k * T))
Rho <- k_1 * (1 / (k_2 - 1))
E <- Rho * lambda_change * v

print(Rho)
print(E)
```

R code Exa 17.15 Evaluating coefficient of integral in formula

```r
# Page 482

h <- 6.626 * 10^-34
pi <- 3.1415
m <- 9.1094 * 10^-31

c <- (4 * pi * (2 * m)^1.5) / h^3

print(c)
```

Chapter 18

Reaction Rate Theory

R code Exa 18.6 Estimating the maximum kinetic isotope effect

```
# Page 493

k1 <- 3300
Mu1 <- 1.007825
Mu2 <- 2.0140
e <- 2.71828
k <- 0.69504
T <- 298.15

lambda <- (1/2) * k1 * (1 - sqrt(Mu1 / Mu2))
k2_k1 <- exp(-lambda / (k * T))
k1_k2 <- 1 / k2_k1

print(k2_k1)
print(k1_k2)
```

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

```r
# Page 503

k <- 1.76 * 10^13
h <- 6.62608 * 10^-34
kb <-  1.38066 * 10^-23
T <- 202.50
e <- 2.71828
R <- 8.31451
E_a <- 46860

k_1 <- (e * ((kb * T) / h))
K <- k / k_1
S <- R * log (K)
H <- E_a - (R * T)
G <- H - (T * S)

print(S)
print(H)
print(G)

# 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

```
# Page 510

I1_I0 <- 0.727
I2_I1 <- 0.407

I2_I0 <- I1_I0 * I2_I1

print(I2_I0)
```

R code Exa 19.3 Calculating the photon energy

```
# Page 512

e <- 1.6 * 10^-19
E_photon <- 1 * 10^-3
c <- 2.99792 * 10^8
M <- 5.6857 * 10^-12
```

```

k <- 2 * M * c^2
E <- k * E_photon * e

print(E)
```

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

```
# Page 514

I_I0 <- 0.160
l <- 0.100
B <- 0.0500

A <- -log10(I_I0)
E <- A / (B * l)

print(A)
print(E)
```

R code Exa 19.5 Evaluate the product N X h X c

```
# Page 514

h <- 6.62608 * 10^-34
c <- 2.99792 * 10^8
N <- 6.022 * 10^23

k <- N * h * c

print(k)
```

R code Exa 19.6 Calculating oscillator strength

```r
# Page 515

k <- 1.0645
k_1 <- 4.32 * 10^-9
e_max <- 44000
v <- 5000

K <- k * e_max * v
f <- K * k_1

print(K)
print(f)
```