Corrections to Quantum Chemistry and Spectroscopy

Correction to Chapter 2

Equation 2.33 should read

\[ f(x) = \left( 50 \left( \frac{x}{b} \right)^2 - 1 \right) e^{-\frac{25x^2}{2b^2}} \quad -1 \leq \frac{x}{b} < 1 \]

\[ f(x) = f(x - 2b) \text{ for all } x \]

Correction to Chapter 7

p. 111 The zero line in Figure 7.6 is incorrectly placed. Please use the figure below:
Corrections to Chapter 8

p. 138 The right-hand labels for the three graphs are incorrect in Figure 8.7. Please use the figure supplied below:

![Graphs with corrected labels](image)

p. 139 The last equation on this page should read

\[
l = -\frac{1}{Me(\lambda)} \ln \left( \frac{I(\lambda)}{I_0(\lambda)} \right) = -\frac{1}{40 \text{ (cm bar)}^{-1}(2.0 \times 10^{-6} \text{ bar})} \ln 0.90 = 1.3 \times 10^3 \text{ cm}
\]
Corrections for Chapter 9:

p. 174 The text for the Solution of Example Problem 9.6 on this page should read as follows:

The radial distribution function is

\[ P(r) = r^2 R^2(r) = \frac{1}{8} \left( \frac{1}{a_0} \right)^3 r^2 \left( 2 - \frac{r}{a_0} \right)^2 e^{-r/a_0} \]

To find the maxima, we plot \( P(r) \) and

\[ \frac{dP(r)}{dr} = \frac{r}{8a_0^5} (8a_0^3 - 16a_0^2 r + 8a_0 r^2 - r^3) e^{-r/a_0} \]

versus \( r/a_0 \) and look for the nodes in this function. These functions are plotted as a function of \( r/a_0 \) in the following figure:

p. 178 The first term of the equation for P9.10 should be deleted, and the equation should read:

\[ -\frac{\hbar^2}{2\mu r^2} \frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] + \left[ \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{e^2}{4\pi \varepsilon_0 r} \right] R(r) \]

\[ = E R(r) \text{ for } l = 1 \]
Corrections for Chapter 10:

p. 208 The y-axis captions of the radial probability distribution figures, part (c) of Q10.11 through Q10.18, are incorrect.
to 210 Please use the following corrected figures:
(a) 

(b) 

(c) 

Q10.14
Correction to Chapter 12:

p. 245 In P12.2, the cross-reference should be to Equation (12.7).
Correction to Chapter 14:

p. 288 The artwork for Figure 14.13 is incorrect. Please use the following:

![Visual representation of corrected artwork](image)

Correction to Chapter 15:

p. 305 In Table 15.1 the electron configuration is incorrect for N$_2^+$. The correct listing is

$$(1o_g^1)^2 (1o_u^*)^2 (2o_g^2)^2 (2o_u^*)^2 (1\pi_u^2)^2 (1\pi_u^*)^2 (3\sigma_g^1)^1$$

Corrections to Chapter 16:

p. 355 Equation (16.59) is incorrect. It should read

$$q_{\mu} = P_{\mu\mu} + \sum P_{\mu\nu} S_{\nu\nu}$$

Equation (16.61) is incorrect. It should read

$$Q_A = Z_A - q_A$$

p. 361 The caption for Figure 16.29 should read

The **LUMO** (left) and **HOMO** (right) for acetone identify regions where electrophilic and nucleophilic attack, respectively, are likely to occur.
Corrections for Chapter 17:

p. 404 Equation (17.22) should read

\[ n_i = \frac{1}{\hbar} \Gamma_i \Gamma_{\text{reducible}} = \frac{1}{\hbar} \chi_i (\mathbf{r}_j) \cdot \chi_{\text{reducible}} (\mathbf{r}_j) = \frac{1}{\hbar} \sum_{j=1}^{n} \chi_i (\mathbf{r}_j) \chi_{\text{reducible}} (\mathbf{r}_j), \quad i = 1, 2, \ldots, N \]

p. 410 The caption for Figure 17.11 should read

The ethene MO that is a basis of the $B_{1u}$ representation.