Corrections for *Quantum Theory for Chemical Applications*

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This file will be updated as needed. Corrections listed are based on the first set of prints from early 2021. Some corrections may have been applied by the publisher in the meantime.

Page 36, seven lines below Eq. (3.15), $\hat{x} = i\hbar(\partial/\partial x)$ should read $\hat{x} = i\hbar(\partial/\partial p_x)$

Page 37, after the second display equation, delete the word 'curly'

Page 110, line 4 below Fig. 7.1: after 'modern formulation', replace the period by a comma

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Page 110, last line of display equation at bottom of page: In the numerator, replace x_1 by $x_2 - x_1$

Page 130, line 5: After 'orbitals 1 and 2', replace 'and' by 'are'

Page 131, line 4: After 'antisymmetrizers, differ', 'my' should read 'by'

Page 149: Exercise 8.1 is missing an asterisk indicating that a solution is available in the Appendix.

Page 165: The display equation near the bottom of the page should read (ζ was missing in the argument of the last exponential):

$$\chi_{\alpha/\beta} = \sqrt{\frac{\zeta^3}{\pi}} e^{-\zeta|\boldsymbol{r}-\boldsymbol{R}_{A/B}|} = \sqrt{\frac{\zeta^3}{\pi}} e^{-\zeta r_{A/B}}$$

Page 256, line 7 (counting the unnumbered figure as one line): After 'there is a sign', replace 'chain' by 'change'.

Page 268, first line after Figure 13.16: After 'qualitatively, as', insert '1s or 2s'. Should read: 'qualitatively, as 1s or 2s orbitals'

Chapter 10: In Figure 10.5, 10.6, 10.12, and 10.13, the isosurface values of ± 0.03 au given in the first line of the caption should be changed to ± 0.04 au.

Page 334, Table 17.1: In the radial function for $n = 3, \ell = 0$, delete the factor of 2 before the exponential function. The expression should read

$$\frac{2}{3}\sqrt{\frac{Z^3}{3}}e^{-\frac{rZ}{3}}\left(\frac{2r^2Z^2}{27} - \frac{2rZ}{3} + 1\right)$$

Page 458: Near the top of the page, in the first display equation, inside the square brackets $E^{(0,1)}$ is missing a subscript i. The equation should read

$$e^{-E_i/(k_BT)} = e^{-E_i^{(0,0)}/(k_BT)}\left[1 - \frac{E_i^{(0,1)}}{k_BT}\lambda_2 + \dots\right]$$