

**Corrections for March 2006 reprinting of 2nd Edition of
*Essentials of Computational Chemistry – C. J. Cramer***

January 17, 2007

1. Page 38. Change eq. (2.30) as below

$$\sigma_{AB} = \frac{1}{2}(\sigma_A + \sigma_B) \quad (2.30)$$

2. Page 107. Change eq. (4.3) as below

$$H = - \sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_k \frac{\hbar^2}{2m_k} \nabla_k^2 - \sum_i \sum_k \frac{e^2 Z_k}{4\pi\epsilon_0 r_{ik}} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0 r_{ij}} + \sum_{k<l} \frac{e^2 Z_k Z_l}{4\pi\epsilon_0 r_{kl}} \quad (4.3)$$

and change the sentence fragment immediately underneath the equation to: where i and j run over electrons, k and l run over nuclei, \hbar is Planck's constant divided by 2π , m_e is the mass of the electron, m_k is the mass of nucleus k , ∇^2 is the Laplacian operator, e is the charge on the electron, Z is an atomic number, ϵ_0 is the permittivity of free space, and r_{ab} is the distance between particles a and b .

3. Page 163. The following citation should be added to the references: Dewar, M. J. S. and Thiel, W. 1977. *J. Am. Chem. Soc.*, **99**, 4899.

4. Page 214: Change eq. (7.16) as below

$$E = \frac{1}{2} \left[H_{11} + H_{22} \pm \sqrt{(H_{22} - H_{11})^2 + 4H_{12}^2} \right] \quad (7.16)$$

5. Page 215, line 7: Change “size consistent” to “size-extensive”

Page 215, 6 lines below eq. (7.18): Change “-consistent” to “-extensive”

Page 221, 3 lines from bottom: Change “-consistent” to “-extensive”

Page 225, 6 lines below eq. (7.54): Change “-consistent” to “-extensive”

Page 225, 7 lines below eq. (7-54): Change “consistency” to “extensivity”

Page 226, 15 lines below eq. (7.56): Change “-consistency” to “-extensivity”

Page 226, last line: Change “inconsistency” to “non-extensivity”

Page 257, 4 lines above Section 8.4: Change “-consistent” to “-extensive”

6. Page 255. Change eq. (8.16) as below

$$\rho(\mathbf{r}) = \sum_{i=1}^N |\chi_i(\mathbf{r})|^2 \quad (8.16)$$

7. Page 270: Change eq. (8.40) as below

$$\delta\rho(\mathbf{r}) = \sum_A^{\text{atoms}} \Delta q_A(\mathbf{r}) \quad (8.40)$$

8. Page 295, 6th reference in rightmost table column: page number should be “11623” instead of “623”

9. Page 310, 4 lines above eq. (9.7): Change “Marsilli” to “Marsili”
Page 352, 20th reference: Change “Marsilli” to “Marsili”

10. Page 539. Change eq. (15.42) as below

$$\Psi(\mathbf{Q}, \mathbf{q}) = c_1(\mathbf{Q})\psi_1(\mathbf{q}; \mathbf{Q}) + c_2(\mathbf{Q})\psi_2(\mathbf{q}; \mathbf{Q}) \quad (15.42)$$