Corrections for January 2008 reprinting of 2nd Edition of

Essentials of Computational Chemistry – C. J. Cramer

November 10, 2009

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

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

2. Page 43, line above eq. (2.34): Change "Differentiation of *E*" to "Differentiation of *U*".

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

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_k \frac{\hbar^2}{2m_k}\nabla_k^2 - \sum_i \sum_k \frac{e^2 Z_k}{4\pi\varepsilon_0 r_{ik}} + \sum_{i<j} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{k<l} \frac{e^2 Z_k Z_l}{4\pi\varepsilon_0 r_{kl}} \tag{4.3}$$

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*.

4. 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.

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

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

6. 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"

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

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

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

$$\delta\rho(\mathbf{r}) = \sum_{\mathrm{A}}^{\text{atoms}} \Delta q_{\mathrm{A}}(\mathbf{r}) \tag{8.40}$$

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

10. Page 310, 4 lines above eq. (9.7): Change "Marsilli" to "Marsili"

Page 352, 20th reference: Change "Marsilli" to "Marsili"

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

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