J|A|C|S
ADDITIONS AND CORRECTIONS

Proton-Coupled Electron Transfer in a Model for Tyrosine Oxidation in Photosystem II [*J. Am. Chem. Soc.* **2003,** *125,* 10429–10436]. Claudio Carra, Nedialka Iordanova, and Sharon Hammes-Schiffer*

Page 10431. One of the parameters in the gas phase empirical valence bond (EVB) potential for the proton-coupled electron transfer reaction was inadvertently given incorrectly. In the gas phase EVB potential, the O_A-O_D distance was 2.364 Å rather than the previously reported value of 2.63 Å, which was the distance used in the calculations of the solvation and reorganization energies. Since the coupling V^{PT} in the gas phase EVB potential was fit to the experimental rate at pH = 7, the O_A-O_D distance can be viewed as a parameter in the empirical potential. If a longer O_A-O_D distance were used in the gas phase EVB potential, typically a larger value of V^{PT} would be required to reproduce the same experimental rate, but the qualitative analysis would not be altered. This reporting error for a single parameter does not impact the results and conclusions.

JA803574N

10.1021/ja803574n
Published on Web 06/03/2008

10.1021/ja803574n CCC: $40.75