

Erratum for:

Molecular Modeling of Environmentally Important Processes: Reduction Potentials. Lewis, A.; Bumpus, J. A.; Truhlar, D. G.; Cramer, C. J. *J. Chem. Educ.* **2004**, *81*, 596-603

On page 597 we incorrectly stated that the free energy of solvation of the proton, -1104.5 kJ/mol, reported by Tissandier et al. (1) in 1998, corresponds to the same concentration in the gas phase and in liquid solution. Actually, their reported result corresponds to the standard state of 1 atm in the gas phase and 1 M in solution. Therefore it is not appropriate to make any correction to their measured value, as was done in our article to arrive at a 1 atm to 1 M transfer free energy of -1096.6 kJ/mol.

Nevertheless, we consider our numbers to remain essentially correct because in 2002 Zhan and Dixon (2) reported an updated value for the 1 atm to 1 M proton solvation free energy of -1097.9 kJ/mol that (fortuitously) agrees with the value (-1096.6 kJ/mol) that we used to within their error bars of 4.2 kJ/mol. In Table 2, converting our value to hartrees gives -0.41766 , whereas converting theirs (2) gives -0.41816 ± 0.00159 hartrees. Tissandier et al. (1) reported an even larger uncertainty (8.4 kJ/mol = 0.00319 hartrees) associated with their value. Thus, the value that we used is well within the uncertainty of the two best values in the literature and should still be considered to be accurate.

1. Tissandier, M. D.; Cowen, K. A.; Feng, W. Y.; Gundlach, E.; Cohen, M. H.; Earhart, A. D.; Coe, J. V.; Tuttle, T. R. *J. Phys. Chem. A* **1998**, *102*, 7787-7794.
2. Zhan, C.-G.; Dixon, D. A. *J. Phys. Chem. A* **2001**, *105*, 11534-11540.