Erratum: "Density functional solvation model based on CM2 atomic charges" [J. Chem. Phys. 109, 9117 (1998); 111, 5624 (E) (1999)]

Tianhai Zhu, Jiabo Li, Gregory D. Hawkins, Christopher J. Cramer, and Donald G. Truhlar

Citation: The Journal of Chemical Physics **113**, 3930 (2000); doi: 10.1063/1.1286968
View online: http://dx.doi.org/10.1063/1.1286968
View Table of Contents: http://aip.scitation.org/toc/jcp/113/9
Published by the American Institute of Physics

Erratum: ''Density functional solvation model based on CM2 atomic charges'' [J. Chem. Phys. 109, 9117 (1998); 111, 5624 (E) (1999)]

Tianhai Zhu, Jiabo Li, Gregory D. Hawkins, Christopher J. Cramer, and Donald G. Truhlar
Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, Minnesota 55455-0431

[S0021-9606(00)00832-1]

There are several typos in Table II. For the DZVP basis, $\sigma_{HN}^{(n)}(2)$ should be -183.60, not -188.51. For the 6-31G* basis, $\sigma_{I}^{(water)}$ should be -22.63, not -23.63, $\sigma_{HN}^{(water)}(2)$ should be -207.7, not $+199.86$, and $\sigma_{HO}^{(water)}(2)$ should be 451.65, not 139.93. Finally, P,O and P,S should be O,P and S,P, respectively. These are all typos and do not affect any results.

We are grateful to Laura Masgrau, Paul Winget, and James Xidos for assistance in checking all parameters.

