ADDITIONS AND CORRECTIONS

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R. Schurhammer and G. Wipff: Are the Hydrophobic $AsPh_4^+$ and BPh_4^- Ions Equally Solvated? A Theoretical Investigation in Aqueous and Nonaqueous Solutions Using Different Charge Distributions

Page 11168. **Note Added in Proof.** We tested the recently published TIP5P water model of W. L. Jorgensen et al.,[57] in which the negative charge is borne by two lone pairs instead of the oxygen center. MD was run using an 11 Å cutoff and the RF correction. The TIP5P model solves a number of problems. The electrostatic potential $\phi(S^0)$ at the center of a neutral sphere S^0 (defined by $R^* = 5.5$ Å and $\epsilon = 0.1$ kcal/mol as in ref 12) is now close to zero (+0.9 kcal/mol), instead of +9 kcal/mol with the TIP3P-like models. According to the RDFs, this results from equidistant first shell lone pairs and proton charges, which make closer contacts with S^0 than do the oxygen atoms. The TIP5P water model thus reduces the difference between the ΔG^{0+} and ΔG^{0-} free energies of charging, compared to TIP3P or SPC models. Indeed, for charging the neutral sphere S^0, ΔG^{0+} and ΔG^{0-} are −14.2 and −17.4 kcal/mol, respectively, in TIP5P water, instead of −6.3 and −27.3 kcal/mol in TIP3P water. For the tetrahedral $AsPh_4^0$ or BPh_4^0 species (*set 8* charges), ΔG^{0+} and ΔG^{0-} are −16.0 and −19.9 kcal/mol, respectively, in TIP5P water. This leads to a ΔG^{+-} difference of free energies of hydration of −4.3 kcal/mol, i.e., much less than the corresponding TIP3P value of −21.2 kcal/mol. The percentage of TIP5P bridging water molecules remains larger, around BPh_4^- (10%) than $AsPh_4^+$ (0%), which contributes to the better hydration of the anion. It thus seems that the TATB problem is particularly suitable to test water models and related hydrophilic/hydrophobic interactions.

Page 11161. In Table 1, *Handmade* refers to *set6*, *set7*, *set8*.

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