Additions and Corrections

Quantum Chemical Analysis of *para*-Substitution Effects on the Electronic Structure of Phenylnitrenium Ions in the Gas Phase and Aqueous Solution [*J. Am. Chem. Soc.* **1998**, *120*, 11778−11783]. MICHAEL B. SULLIVAN, KENNETH BROWN, CHRISTOPHER J. CRAMER,* AND DONALD G. TRUHLAR*

Substitution effects on singlet−triplet splittings in aqueous solution were partially obscured by incomplete convergence of aqueous solvation free energies. In addition, the gas-phase and solution-phase ρ values were typographically interchanged. Corrected portions of Tables 1 and 5 are provided below and reflect all solvation free energies having been converged to 0.1 kcal/mol. Quantitative changes affect the original paper as follows.

Page 11778, abstract, line 6: $\rho = 6.4$ should read as $\rho = 7.7$.

In the abstract (page 11778), the third paragraph of the discussion (page 11780, right column), and the last paragraph of the conclusions (page 11783, right column), incorrect variations on the following two sentences appear. They should read as follows: In 13 of 15 cases, the singlet is better solvated than the triplet by 0.9−3.7 kcal/mol. For the cases of CN and CF_3, the triplet is better solvated than the singlet, but by only a small amount, 0.6 and 0.8 kcal/mol, respectively.

Page 11780, right column, line 40: 2.1 kcal/mol should read as 1.7 kcal/mol.

Page 11783, left column, line 18: 5.6 (σ^+) to 9.3 should read as 4.6 (σ^+) to 7.7. The paragraph of discussion beginning on line 24 should read as follows: Another feature of the S-T splitting correlations is that they are substantially improved in every case when the regression is on the data for aqueous solution instead of the gas phase. The absolute magnitude of the interaction difference between a *para* substituent and the electron-deficient center in singlets vs triplets is in every case *enhanced* by aqueous solvation, as indicated by larger ρ values in solution than in the gas phase for all three descriptor sets; put differently, the relative charge-donating or -accepting character of substituents is accentuated in aqueous solution.

Table 1E. Corrections to Aqueous Solvation Free Energies (ΔG_s°) and Aqueous S-T Splittings for *para*-Substituted Phenylnitrenium Ions.

para substituent	electronic state	ΔG_s°	S-T splittings
$N(CH_3)_2$	^1A	−53.0	
	$^3A'$	−50.1	−30.7
NH_2	$^3A''$	−57.1	−31.5
OH	^3A	−59.3	−28.4
OCH_3	$^1A'$	−53.6	
	^3A	−51.7	−28.7
CHO	^3A	−55.2	−15.8
CO_2H	^3A	−58.0	−18.0
CO_2CH_3	^1A	−53.1	
	^3A	−51.0	−18.6
$COCH_3$	^3A	−53.1	−15.6
CN	^1A	−60.3	
	^3A	−61.0	−16.9
NO_2	^3A	−58.0	−17.7

Table 5E. Correlation Coefficients R (unitless) for Regression of *para*-Substituted Phenylnitrenium S-T Splittings on σ_p, σ^+, and σ_R^+ Values

property	σ_p	σ^+	σ_R^+
S-T splitting[a]	0.919 (0.834)	0.974 (0.951)	0.960 (0.943)

[a] Values are tabulated as aqueous solution (gas-phase). Corresponding ρ values are 7.7 (6.4), 4.6 (3.8), 5.5 (4.6).

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Experimental and Theoretical Spin Density in a Ferromagnetic Molecular Complex Presenting Interheteromolecular Hydrogen Bonds [*J. Am. Chem. Soc.* **1999**, *121*, 10126-10133]. YVES PONTILLON, TAKEYUKI AKITA, ANDRE GRAND, KEIJI KOBAYASHI, EDDY LELIEVRE-BERNA, JACQUES PÉCAUT, ERIC RESSOUCHE, AND JACQUES SCHWEIZER*

The following Supporting Information paragraph was omitted from this paper.

Supporting Information Available: Tables of atomic coordinates and equivalent isotropic displacement parameters for **1**, bond lengths and angles, anisotropic displacement parameters for **1**, hydrogen coordinates, and x', y', and z' atomic positions and thermal parameters (PDF). This material is available free of charge via the Internet at http://pubs.acs.org.

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