

Correction to “Driving Force Dependence of Charge Recombination in Reactive and Nonreactive Solvents”

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We noticed a few errors and typos in some of the equations in our article. All calculations and simulations have been performed with the correct equations (as outlined below), and therefore, these errors have no consequences on the discussion of the results and the conclusions.

- The reflecting inner boundary conditions on page 9478 should account for the potential of mean force and the coulomb attraction.

$$\left(\frac{\partial n(r, t)}{\partial r} + n(r, t) \frac{\partial \nu(r)}{\partial r} \right) \Big|_{r=\sigma} = 0$$
$$\left(\frac{\partial m(r, t)}{\partial r} + m(r, t) \left(\frac{\partial \nu(r)}{\partial r} - \frac{r_C}{r^2} \right) \right) \Big|_{r=\sigma} = 0$$

- There are two typos in the diffusion operator (eq 8), which should read

$$\hat{L}_x = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 D(r) \exp(-\nu_x(r)) \frac{\partial}{\partial r} \exp(\nu_x(r))$$

- We take the opportunity to clarify the formulation of eq 18 by adding the subindex x to $w(r)$ and giving the proper subindex, s , to the reorganization energy in the denominator of the exponent. The reorganization energy in the exponent should merely account for the solvent contributions.

$$w_x(r) = \sum_{n=0}^{n=\infty} \frac{U(r) e^{-S} S^n / n!}{1 + \tau_s U(r) e^{-S} S^n / n!} \exp \left(- \frac{(\Delta G_x(r) + \lambda_s(r) + \hbar \omega n)^2}{4 k_B T \lambda_s(r)} \right)$$

- Similarly, the reaction probability in eq 20 should be written as depending on the variables r and t , rather than r and X , as the latter itself is a function of time. Thus, one should replace $w(r, X)$ by $w(r, t)$:

$$w(r, t) = \sum_{n=0}^{n=\infty} U(r) e^{-S} S^n / n! \exp \left(- \frac{(\Delta G(r, t) + \lambda_{cv} + \hbar \omega n)^2}{4 k_B T \lambda_{cv}} \right)$$

- In addition, the units for the resnorm in Table 3 are in ns^{-1} and not in s^{-1} .

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