ADDITIONS AND CORRECTIONS

2004, Volume 108B

Saba M. Mattar*: Role of the Solvent in Computing the 1,4-Benzosemiquinone g-Tensor by the Coupled-Perturbed Kohn—Sham Hybrid Density Functional Method

Page 9452. The correct and complete form of equation 4 should be:

$$\Delta g_{\rm rs}^{\rm OZ/SOC} = -\frac{1}{\beta S} \sum_{\sigma = \alpha, \beta} (-1)^{\delta_{\sigma\beta}} \sum_{i} \sum_{a \in \sigma} \frac{\langle \varphi_{a}^{\sigma(0)} | \beta \zeta_{\rm r} | \varphi_{i}^{\sigma(0)} \rangle}{\epsilon_{a}^{\sigma(0)} - \epsilon_{i}^{\sigma(0)}} \times \left| \varphi_{i}^{\sigma(0)} \right| \sum_{A} \sum_{j} \left[\frac{\alpha^{2}}{2} \frac{Z_{\rm eff}^{A}}{|\vec{r}_{j} - \vec{R}_{A}|^{3}} \right] \zeta_{A, s} \left| \varphi_{a}^{\sigma(0)} \right\rangle$$
(4)

10.1021/jp040763z Published on Web 01/22/2005