ADDITIONS AND CORRECTIONS

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James A. Miller,* Stephen J. Klippenstein, and Struan H. Robertson: A Theoretical Analysis of the Reaction between Vinyl and Acetylene: Quantum Chemistry and Solution of the Master Equation

Page 7527−7528. Although the calculations presented in the paper were performed correctly, there are several errors in the presentation of the theory. Most notably, the partition function $Q_1(T)$ was omitted in several equations in the discussion following eq 9. For clarity we repeat that presentation here, making the appropriate corrections.

Let $x_R(t) = n_R(t)/n_R(0)$, $x_i(E,t) = n_i(E,t)/n_e(0)$, and $y_i(E,t) = x_i(E,t)/f_i(E)$. Then dividing by $n_R(0)f_i(E)$, eq 2 becomes

$$\frac{dy_i(E)}{dt} = Z\int_{E_{oi}}^{\infty}\left\{P_i(E,E')\frac{f_i(E')}{f_i(E)} - \left[1 + \frac{\sum_{j\neq i}^{M} k_{ji}(E) + k_{di}(E)\delta_{i1}}{Z}\right]\delta(E-E')\right\} y_i(E')\,dE' + \sum_{j\neq i}^{M} k_{ij}(E)\frac{f_j(E)}{f_i(E)}y_j(E) + \frac{K_{eqi}}{Q_i(T)}k_{di}(E)\,f_i(E)\,x_R n_m \delta_{i1} - k_{pi}(E)\,y_i(E) \qquad i = 1, ..., M \quad (10)$$

From the detailed balance conditions (8) and (9), one can see that eq 10 is symmetric in E and E' and in i and j. By this we mean that the coefficient of $y_i(E')$ in eq 10 is identical to the coefficient of $y_i(E)$ in an analogous equation for $dy_i(E')/dt$, i.e., for any specific values of E and E'. Likewise, the coefficient of $y_j(E)$ in (10) is the same as the coefficient of $y_i(E)$ in an analogous equation for $dy_j(E)/dt$ for any values of i and j.

Multiplying eq 5 by $(K_{eq1}n_m/Q_1(T))^{1/2}/n_R(0)$, we obtain

$$\frac{d}{dt}\left[\left(\frac{K_{eq1}n_m}{Q_1(T)}\right)^{1/2} x_R\right] = \left(\frac{K_{eq1}n_m}{Q_1(T)}\right)^{1/2}\int_0^{\infty} k_{d1}(E)\,f_1(E)\,y_1(E)\,dE - x_R\left(\frac{K_{eq1}n_m}{Q_1(T)}\right)^{3/2}\int_0^{\infty} k_{d1}(E)\,f_1^{\,2}(E)\,dE \quad (11)$$

Approximating the integrals in eq 11 as sums and rearranging,

$$\frac{d}{dt}\left[\left(\frac{K_{eq1}n_m}{Q_1(T)\delta E}\right)^{1/2} x_R\right] = \sum_{l=1}^{N_1} y_1(E_l)\left(\frac{K_{eq1}n_m}{Q_1(T)}\delta E\right)^{1/2} f_1(E_l)\,k_{d1}(E_l) - x_R\left(\frac{K_{eq1}n_m}{Q_1(T)}\right)^{3/2}(\delta E)^{1/2}\sum_{l=1}^{N_1} k_{d1}(E_l)\,f_1^{\,2}(E_l) \quad (12)$$

where N_1 is the number of grid points in the energy space of well 1 and δE is the spacing between grid points. Similarly, if we write eq 10 as a sum, the next-to-last term in the component equation for $dy_1(E_l)/dt$ can be written as

$$\left(\frac{K_{eq1}n_m}{Q_1(T)\delta E}\right)^{1/2} x_R\left[\left(\frac{K_{eq1}n_m}{Q_1(T)}\delta E\right)^{1/2} f_1(E_l)\,k_{d1}(E_l)\right] \quad (13)$$

Now the coefficient of $y_1(E_l)$ in eq 12 is the same as that of $(K_{eq1}n_m/Q_1(T)\delta E)^{1/2}x_R$ in (13).

Then the vector of unknowns becomes

$$|w(t)\rangle \rightarrow \left[y_1(E_{01}), ..., y_1(E_l), ..., y_i(E_{0i}), ..., y_i(E_l), ..., \left(\frac{K_{eq1}n_m}{Q_1(T)\delta E}\right)^{1/2} x_R\right]^T$$

We apologize if this has caused any inconvenience.

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Karol Jackowski,* Marcin Wilczek, Magdalena Pecul, and Joanna Sadlej: : Nuclear Magnetic Shielding and Spin-Spin Coupling of 1,2-^{13}C-Enriched Acetylene in Gaseous Mixtures with Xenon and Carbon Dioxide

Page 5956. In the caption for Figure 1, the absolute shielding of liquid TMS should be $\sigma[\mathrm{Si}(\mathit{C}\mathrm{H_3})_4] = 186.37$ ppm and $\sigma[\mathrm{Si}(\mathrm{C}\mathit{H}_3)_4] = 32.775$ ppm.

Page 5956. In lines 4 and 5 of column two should be σ(liq TMS) − $\sigma_0(\mathit{C}\mathrm{O}) = 185.77$ ppm and σ(liq TMS) − $\sigma_0(\mathrm{C}\mathit{H}_4) = 2.164$ ppm.

Page 5957. In line 11 of column one "^1J (^{29}Si^{19}F) in SF_6" should read "^1J(^{29}Si^{19}F) in SiF_4".

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