

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

$$\frac{dy_i(E)}{dt} = Z \int_{E_{oi}}^{\infty} \left\{ P_i(E,E') \frac{f_i(E')}{f_i(E)} - \left[ 1 + \frac{\sum_{j \neq i}^M k_{ji}(E) + k_{di}(E)\delta_{i1}}{Z} \right] \delta(E - E') \right\} y_i(E') dE' + \sum_{j \neq i}^M k_{ij}(E) \frac{f_j(E)}{f_i(E)} y_j(E) + \frac{K_{eqi}}{Q_1(T)} k_{di}(E) f_i(E) x_R n_m \delta_{i1} - k_{pi}(E) y_i(E) \quad i = 1, \dots, M \quad (10)$$

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  $\delta E$  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

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

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-<sup>13</sup>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  $\sigma[\text{Si}(\text{CH}_3)_4] = 186.37$  ppm and  $\sigma[\text{Si}(\text{CH}_3)_4] = 32.775$  ppm.

Page 5956. In lines 4 and 5 of column two should be  $\sigma(\text{liq TMS}) - \sigma_0(\text{CO}) = 185.77$  ppm and  $\sigma(\text{liq TMS}) - \sigma_0(\text{CH}_4) = 2.164$  ppm.

Page 5957. In line 11 of column one “<sup>1</sup>J (<sup>29</sup>Si<sup>19</sup>F) in SF<sub>6</sub>” should read “<sup>1</sup>J(<sup>29</sup>Si<sup>19</sup>F) in SiF<sub>4</sub>”.

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