COMMENTS

Comment on "Initiation and Abstraction Reactions in the Pyrolysis of Acetone"[1]

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In the course of a subsequent investigation, it has been found that product concentrations, measured at room temperature by gas chromatography in previous work in this laboratory, were not converted to concentrations at the reaction temperatures. Accordingly, the rates of product formation and values of k_1 in Figures 1, 5, and 6 and Tables 1−3 should be multiplied by 298 K and divided by the reaction temperatures T. The values of k_5/k_3^2 in Tables 1−3 and Figure 3 should be multipled by T/298 K. The values of k_3 in Table 3 should be multiplied by $(298\ \mathrm{K}/T)^{1/2}$. The Arrhenius expression for the high-pressure limit of k_1 becomes $10^{16.8\pm0.8}\ \mathrm{s}^{-1}\ \exp(-341 \pm 14\ \mathrm{kJ\ mol}^{-1}/RT)$. For reaction 3, the average transitional vibrational term value in the transition state becomes $344 \pm 10\ \mathrm{cm}^{-1}$, the effective activation barrier height, $41 \pm 1\ \mathrm{kJ\ mol}^{-1}$, and the full thickness of the barrier at half height, 63 ± 5 pm. Reaction 3 does not follow the Arrhenius law, but within the temperature range used, the following Arrhenius expression has been fit to the results for k_3: $10^{10.5\pm0.2}\ \mathrm{L\ mol}^{-1}\ \mathrm{s}^{-1}\ \exp(-69 \pm 4\ \mathrm{kJ\ mol}^{-1}/RT)$.

References and Notes

(1) Mousavipour, S. H.; Pacey, P. D. *J. Phys. Chem.* **1996**, *100*, 3573−3579.

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