ADDITIONS AND CORRECTIONS

2008, Volume 112A

Chenlai (Ryan) Zhou, Karina Sendt,* and Brian S. Haynes: Theoretical Study of Hydrogen Abstraction and Sulfur Insertion in the Reaction $H_2S + S$

Page 3239. In our recent paper, a symmetry factor of 2 was incorrectly assigned to TS1 (C_s) in the calculation of the rate constant for the triplet abstraction channel $H_2S + S \rightarrow SH + SH$. Using the correct symmetry factor of 1, the previously reported three-parameter Arrhenius expression should be multiplied by a factor of 2 to give

$$k_{\text{abstraction}} = 7.4 \times 10^6 T^{2.297} \times \exp(-37.7 \text{ kJ mol}^{-1}/RT) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$$

Consequently, the estimate of the rate constant of the insertion channel becomes

$$k_{\text{ins}} = 2.2 \times 10^{13} \exp(-26.2 \text{ kJ mol}^{-1}/RT) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$$

The corrected results do not affect the discussions and conclusions in the original paper, and they are within the uncertainty (a factor of 3) of the adopted theoretical methods.

10.1021/jp810800a
Published on Web 12/31/2008