Study of the Heμ + H_2 Reaction at Room Temperature: Theory and Measurement

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Muonic helium Heμ is a neutral species with the composition $\alpha^{++}\mu^{-}e^{-}$ which can be regarded as a unique heavy H-atom isotope with mass 4.1 amu. It extends the range of H-atom isotopes for the study of kinetic isotope effects from Mu to Heμ, a remarkable factor of 36 in mass.

We have begun kinetics studies of the reaction

$$\mathrm{He}\mu + \mathrm{H_2} \rightarrow \mathrm{He}\mu\mathrm{H} + \mathrm{H} \qquad (2)$$

as a complement to the earlier study [1] of $\mathrm{Mu} + \mathrm{H_2} \rightarrow \mathrm{MuH} + \mathrm{H}$, which is a seminal reaction with precisely-calculated potential energy surfaces [2].

We here present a preliminary reaction rate constant for reaction (1) measured at 295 K, as well as variational transition state calculations of the same. The figure shows both results, with a measured rate $k = 4.1 \pm 0.7 \times 10^{-16}\,\mathrm{cm^3\,s^{-1}}$ and a calculated value of $2.46 \times 10^{-16}\,\mathrm{cm^3\,s^{-1}}$. Despite the large uncertainty in these initial measurements, there appears to be a discrepancy, perhaps indicating more tunneling in the reaction than the VTST calculations account for.

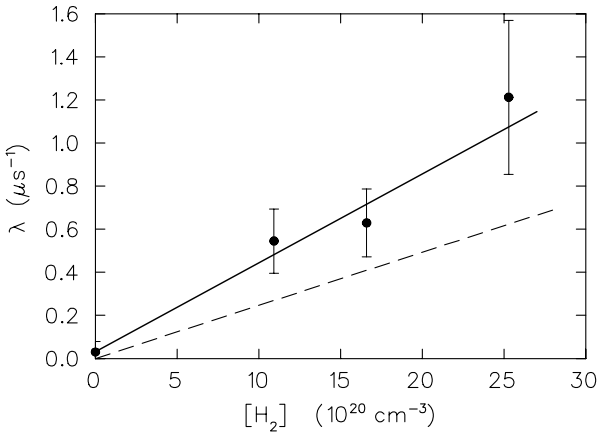

Fig. 1: Reaction rates for the Heμ + H_2 reaction measured (points and solid fitted line) and calculated (dashed line) at 295 K.

[1] I.D. Reid, et al., J. Chem. Phys. **86** 5578 (1987) 5578.
[2] S.L. Mielke, B.C. Garrett and K.A. Peterson, J. Chem. Phys. **116** (2002) 4142.