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Addition/Correction

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Correction to "State-to-State Quantum Mechanical Calculations of Rate Coefficients for the $D^+ + H_2 \rightarrow HD + H^+$ Reaction at Low Temperature"

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A direct comparison of the published time-independent quantum-mechanical (TIQM) result with the statistical quantum-mechanical (SQM) predictions[1] of Tomas Gonzalez Lezana for different values of the asymptotic Jacobi distance R_{max} evidenced that the asymptotic matching hyper-radius ρ_{max} (which is equal to R_{max} at large distance) employed to solve the corresponding coupled second-order differential equations in the hyperspherical adiabatic states was not long enough either.

Here, we present a new Figure 1 and a Table 1 showing, respectively, the $j = 0$ rate coefficient as a function of the collision energy and the temperature dependence of the $j = 0$ rate constant by means of the same TIQM method with a propagation from 0.5 a_0 up to a largest asymptotic matching distance of $\rho_{max} = 40\ a_0$ using the same potential energy surface. In addition, the SQM results presented in the new Figure 1 have been obtained with the parameters reported in ref 1 and the asymptotic R_{max} of 70 a_0.

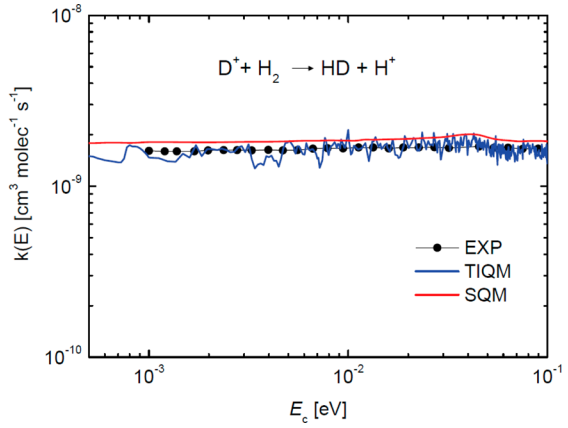

Figure 1. Rate coefficients for the $D^+ + H_2(v = 0, j = 0) \rightarrow HD + H^+$ reaction. TIQM results (blue line) are compared with SQM predictions[1] (red line) and the measurements from ref 23 of the published paper (black circles).

Table 1. TIQM and SQM Rate Constants $k(T)$ in 10^{-9} cm^3·molecule^{-1}·s^{-1}

T, K	SQM	TIQM
10	1.75178	1.35219
20	1.79538	1.48076
30	1.81218	1.53312
40	1.82308	1.56715
50	1.83170	1.59224
60	1.83919	1.61185
70	1.84600	1.62776
80	1.85231	1.64096
90	1.85814	1.65205
100	1.86348	1.66138

The main conclusion is that we find now a very good agreement with Gerlich's experimental results (ref 23 in the published paper), the rate coefficients being nearly constant over all the considered energy range (see the new Figure 1 below). In addition, the TIQM rate constant shown in Figure 5 now presents a much slighter decrease when the temperature decreases (see Table 1 presented below). Figures 2 and 3 are mainly unaffected.

Extended additions and improvements will be given in a future paper with a full comparison with the SQM results, including the differential cross sections and the product energy distributions.

■ ACKNOWLEDGMENTS

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■ REFERENCES

(1) Gonzalez-Lezana, T.; Honvault, P.; Scribano, Y. Dynamics of the $D^+ + H_2$ –> HD + H^+ reaction at the low energy regime by means of a statistical quantum method. *J. Chem. Phys.* **2013**, *139*, 054301.

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