Erratum: Observation of Predicted Resonance Structure in the $H + D_2 \rightarrow HD(v' = 0, j' = 7) + D$ Reaction at a Collision Energy of 0.94 eV [Phys. Rev. Lett. 84, 4325 (2000)]

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DOI: 10.1103/PhysRevLett.86.2482 PACS numbers: 34.50.Pi, 82.20.Pm, 99.10.+g

In our Letter, we reported the observation of resonance structure in the $H + D_2 \rightarrow HD(v' = 0, j' = 7) + D$ reaction at a collision energy of 0.94 eV. The theoretical results in this Letter predicted a resonance near 0.94 eV but were not fully converged with respect to the partial wave sum over the total angular momentum J. However, the experimental data showed intriguing evidence for a resonance at this energy which suggested that it would survive the sum over all partial waves and appear in the fully converged theoretical results. We have recently completed the converged quantum mechanical calculations for this reaction which include all $J \leq 31$ at 64 collision energies between 0.3 and 1.7 eV [1]. Unfortunately, there is no resonance structure for $HD(v' = 0, j' = 7)$ once a fully converged calculation is performed [1,2]. However, resonance structure does survive the partial wave sum in many of the cross sections for $j' < 4$ [1]. Improved experimental techniques might allow for the observation of this structure in the near future.

Figure 1 plots the comparison of the experimental measurements and the theoretical predictions for the title reaction. The thick solid curve is our latest theoretical prediction based on $J \leq 31$ and an off-axis drift parameter (used to model the uncertainty in the experimental instrument function) of $d = 1.5$ mm. The long-dashed curve is the previous theoretical prediction based on $J \leq 6$ and $d = 2.5$ mm [3]. Both of these curves pass through nearly the same number of error bars. The error bars represent one standard deviation of the mean. However, we now see that the excellent agreement between the previous theoretical results for $J \leq 6$ and experiment was fortuitous. No "bump" is found for any value of $d = 0-2.5$ mm using the fully converged results. Although the experimental data is in reasonable agreement with the fully converged theoretical results, the experimental suggestion of a resonance is most likely due to unresolved systematic errors.

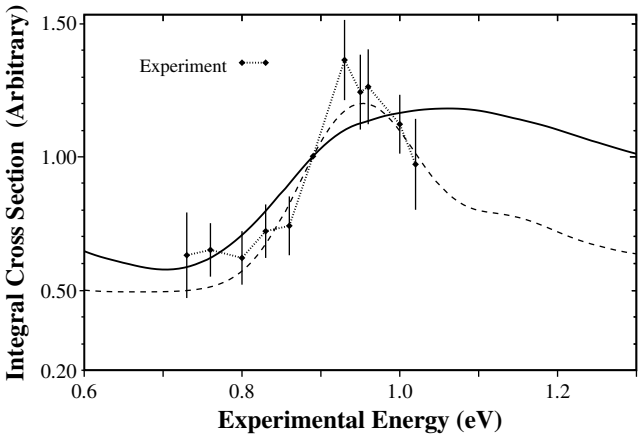

FIG. 1. Comparison of the experimental measurements (solid diamonds) and theoretical predictions for $J \leq 6$ and a misalignment parameter of $d = 2.5$ mm (dashed curve) and for $J \leq 31$ and a misalignment parameter of $d = 1.5$ mm (thick solid curve).

[1] B. K. Kendrick, J. Chem. Phys. (to be published).
[2] We thank F. J. Aoiz, L. Bañares, and J. F. Castillo for bringing the results of their calculations to our attention.
[3] B. K. Kendrick, L. Jayasinghe, S. Moser, M. Auzinsh, and N. Shafer-Ray, Phys. Rev. Lett. **84**, 4325 (2000).

 0031-9007/01/86(11)/2482(1)$15.00