Resonances in the reaction ortho- and para-D$_2$ + H at temperatures below 10 K$^1$ I. SIMBOTIN, R. CÔTÉ, University of Connecticut, Storrs — In a previous study [Simbotin and Côté, New J. Phys. 17, 065003 (2015)] we reported cross sections for the reaction H$_2$ + D in the temperature regime $10^{-6} < T < 10$ K, and found pronounced shape resonances, especially in the $p$ and $d$ partial waves. We found that the resonant structures were sensitive to the initial rovibrational state of H$_2$; in particular, we showed that the effect of the nuclear-spin symmetry was very important, since ortho- and para-H$_2$ gave significantly different results. We now investigate the reaction D$_2$ + H for vibrationally excited ortho- and para-D$_2$, and compare and contrast these results with those for H$_2$ + D. We remark that this benchmark system is a prototypical example of reactions with a strong barrier, which have very small cross sections in the cold and ultracold regimes. However, shape resonances can enhance the reaction cross sections by orders of magnitude for temperatures around and below $T = 1$ K. Moreover, resonant features would provide stringent tests for quantum chemistry calculations of potential energy surfaces.

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