Electronic supplementary information for:

Mode Selective Dynamics and Kinetics of the H_2 + F_2 → H + HF + F Reaction

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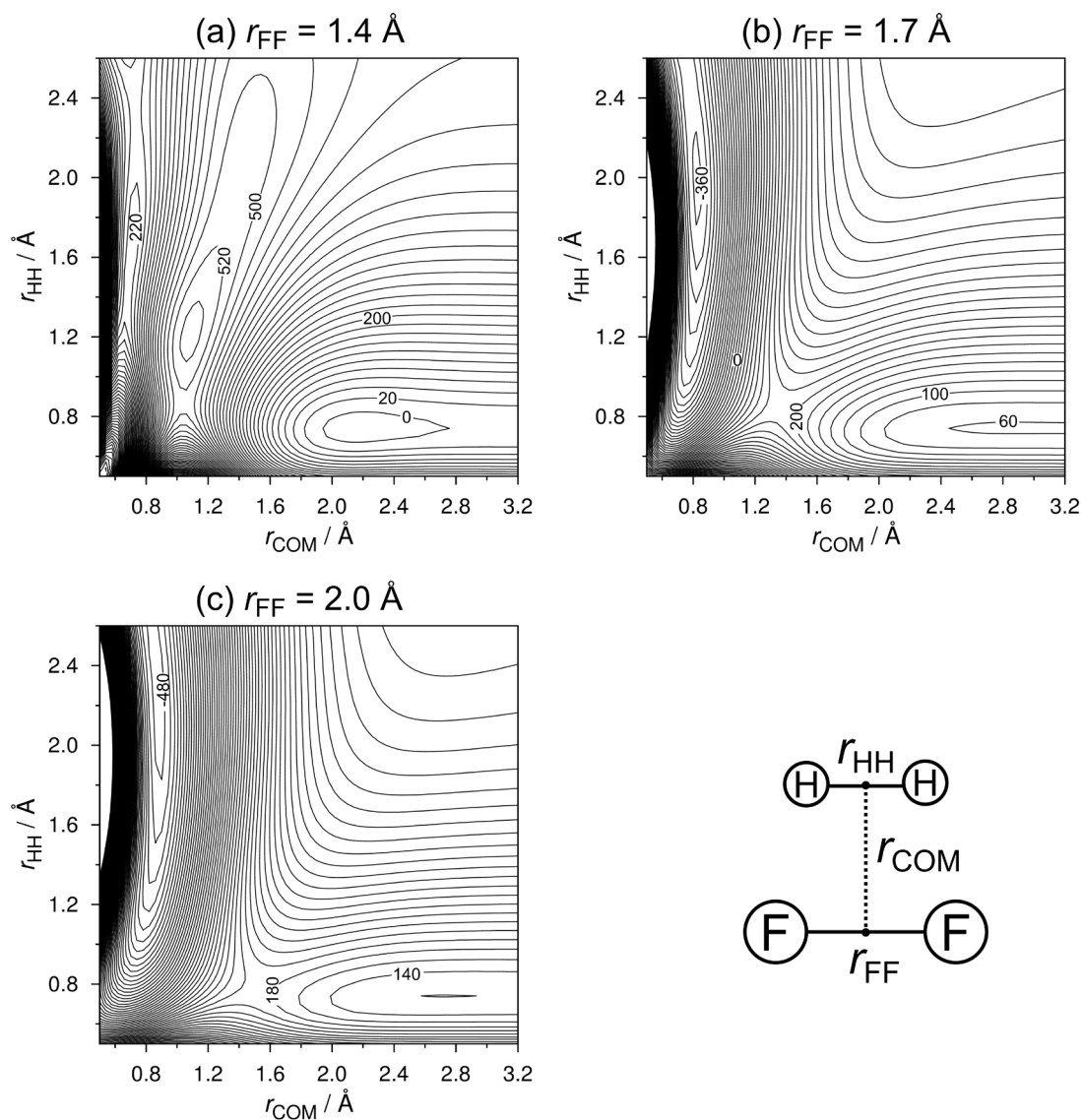
Figure S1. Equipotential contour plots of the $H_2 + F_2$ reaction on the trapezoidal configuration. The contours are plotted as functions of the coordinates r_{COM} and r_{HH} with r_{FF} fixed at 1.4 (a), 1.7 (b), and 2.0 (c) Å. The energies shown are relative to the reactants and the contour increments are 20 kJ mol^{-1}. These contours indicate a potential energy barrier of ~180 kJ mol^{-1} for 2HF channel; however, the saddles shown in the figure are of higher order in the full-dimensional PES, and thus, not representing transition states.
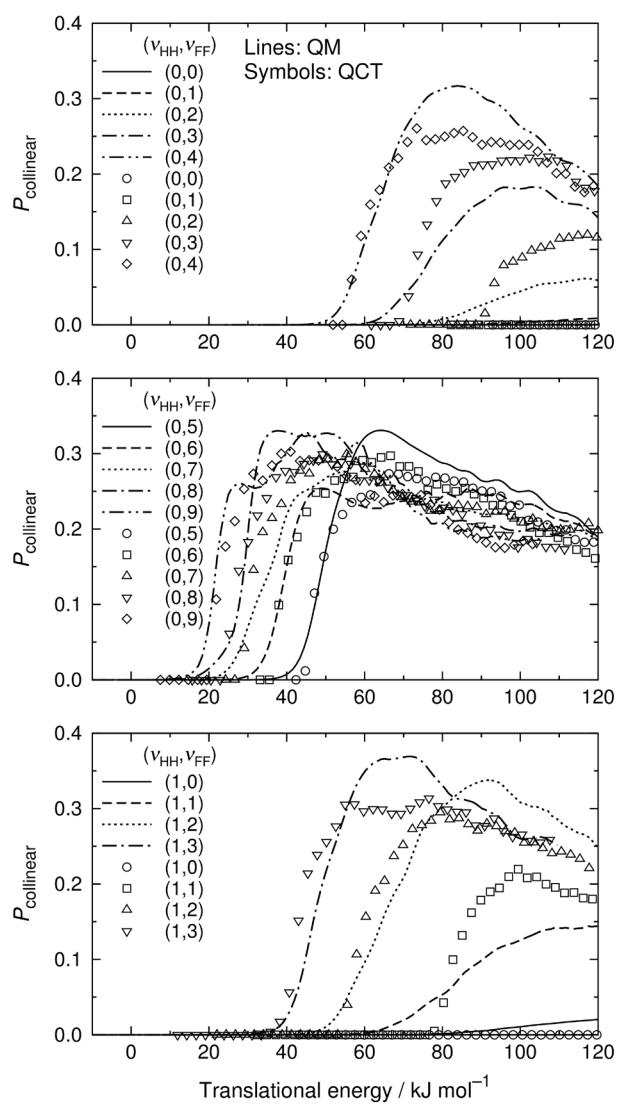
Figure S2. Collinear reaction probabilities for R1 as a function of the relative translational energy.