Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information for:

Dissociation channels, collisional energy transfer, and multichannel coupling effects in the thermal decomposition of CH_3F

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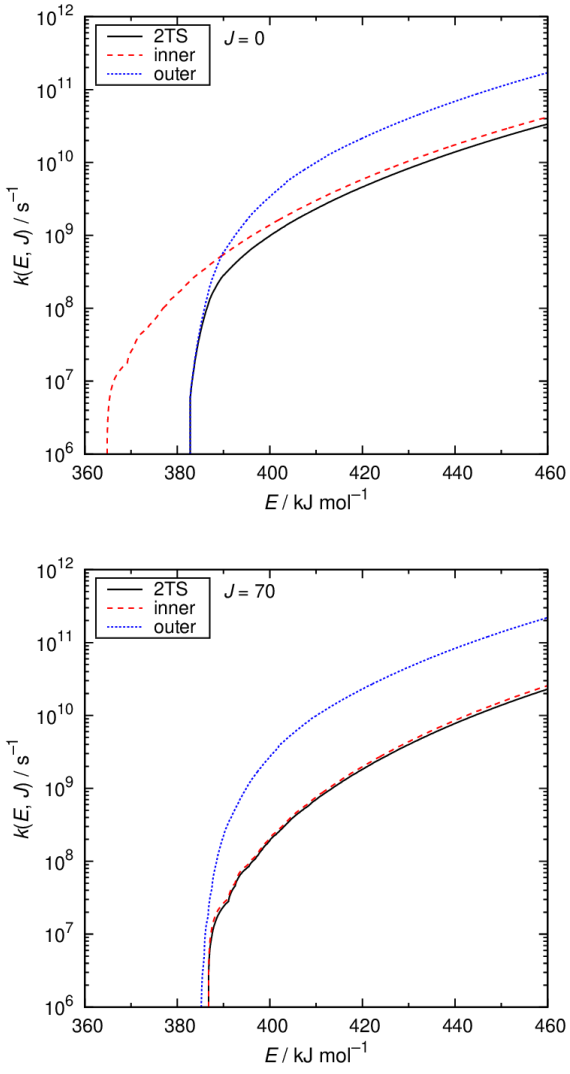

Figure S1. The microcanonical rate constants for the HF elimination channel at $J = 0$ (top) and 70 (bottom) calculated by the two-transition state model (2TS; sloid lines) and those for the inner (dashed lines) and outer (dotted lines) transition states.

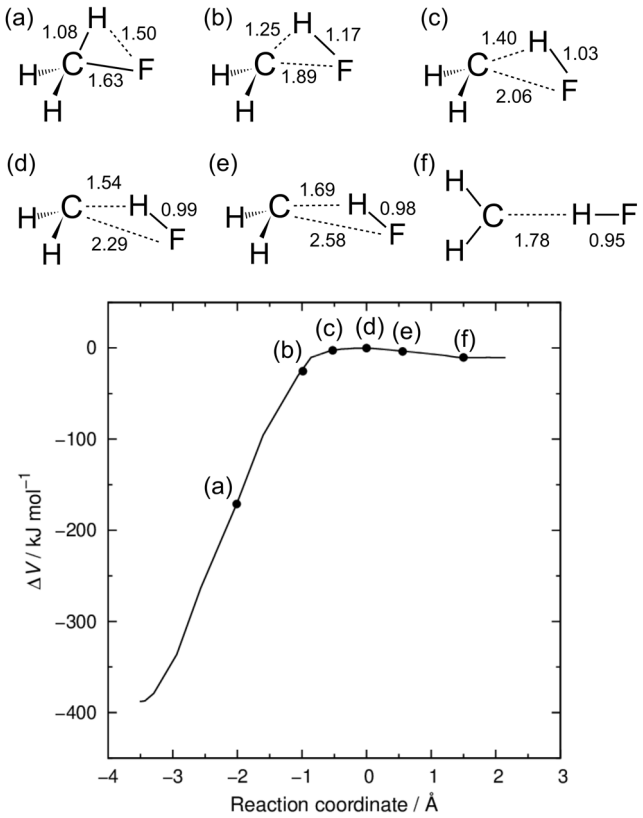

Figure S2. Structural evolution and potential energies (calculated at the ωB97X-D/6-311++G(d,p) level of theory) along the reaction coordinate for the inner transition state of the HF elimination channel. The potential energies plotted are relative to that at the saddle point. Bond lengths are given in angstroms.