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

Supplementary Information for:

Competing quantum effects in the free energy profiles and diffusion rates of hydrogen and deuterium molecules through clathrate hydrates

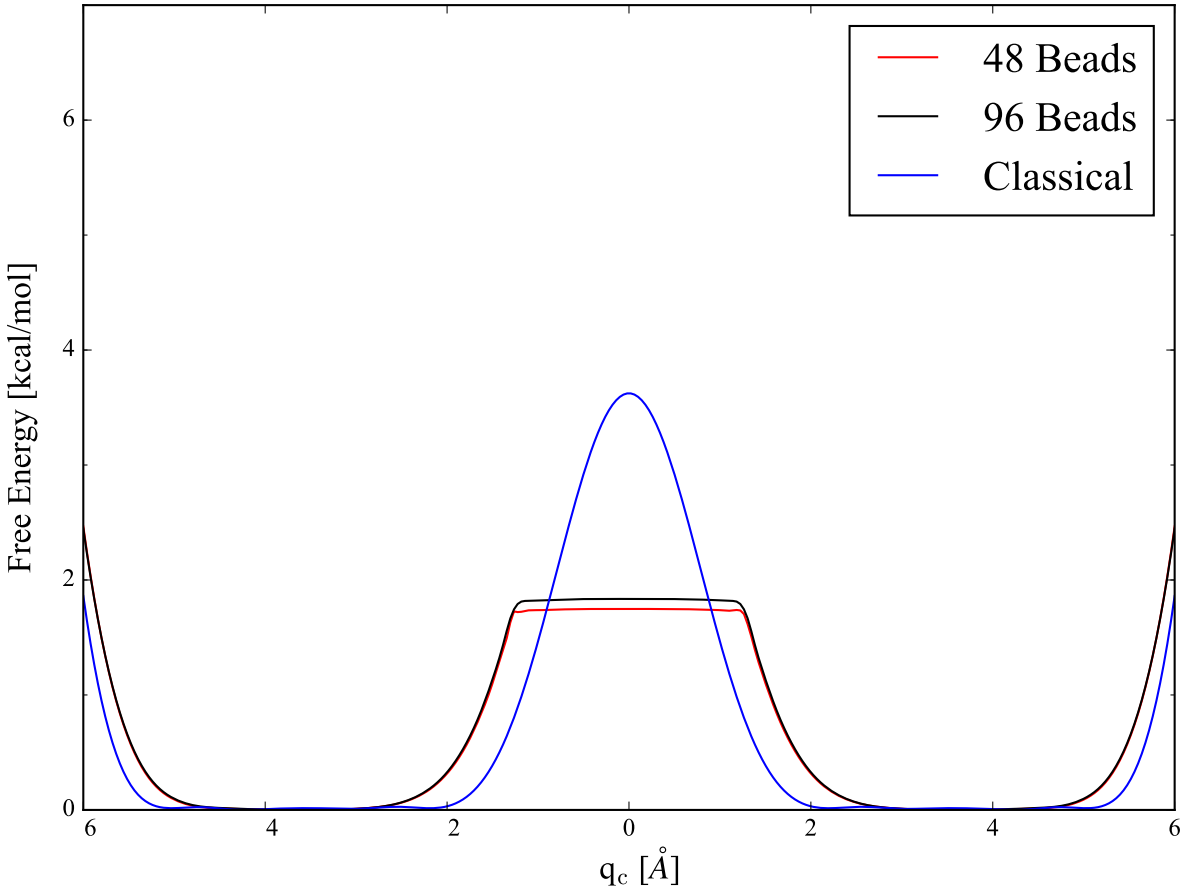

Figure S1. Free energy profiles for hydrogen at 8 K comparing the number of path integral beads. Red corresponds to 48 path integral beads while black represents 96 path integral beads. The blue curve is the classical free energy profile at 8 K. The difference in barrier height between 96 beads and 48 beads is approximately 0.1 kcal/mol, which corresponds to about 5% difference.

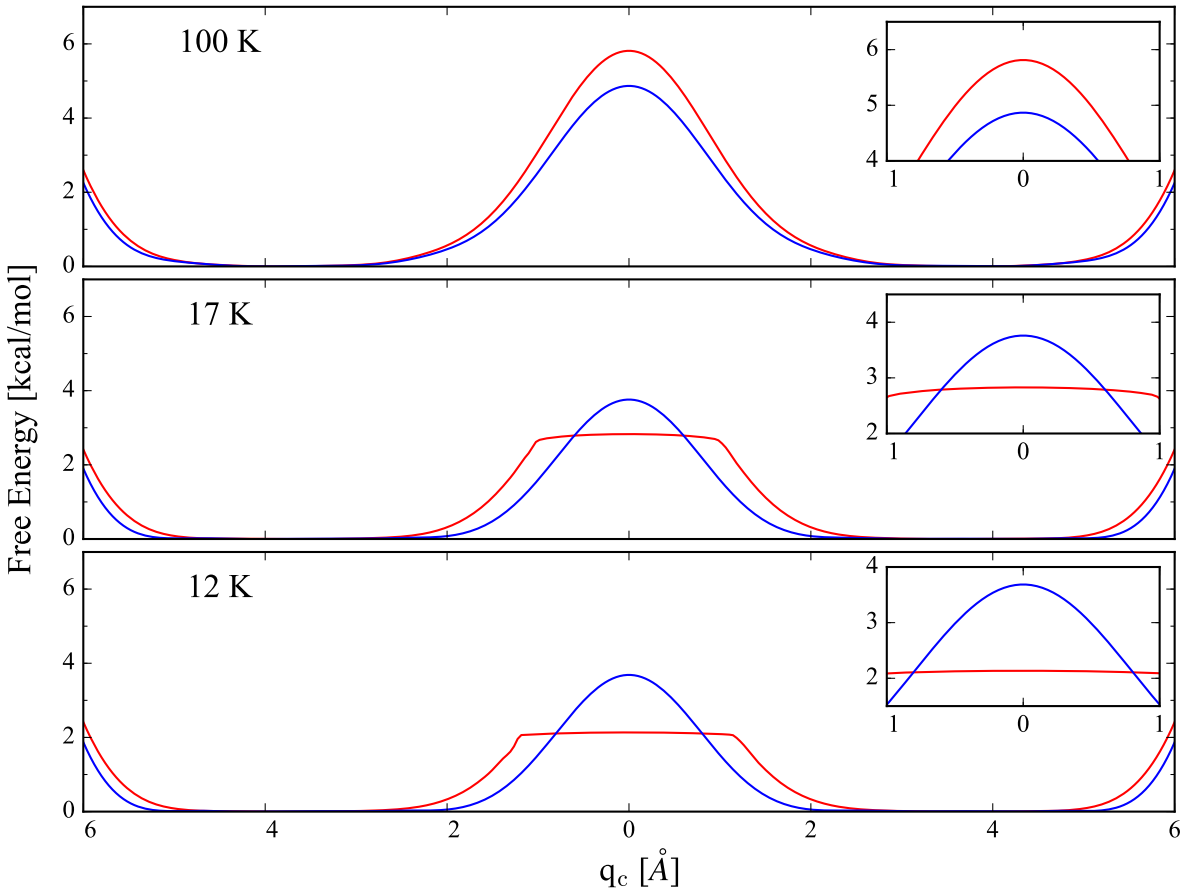

Figure S2. Free energy profiles for a single hydrogen molecule moving through a hexagonal face between two large cages for temperatures of 100K, 17K, and 12K. The H_2 (red) results are from PIMD calculations, which when performed with a single path-integral bead give the classical (blue) free energies. The insets in each plot provide a clearer depiction at the dividing surface.

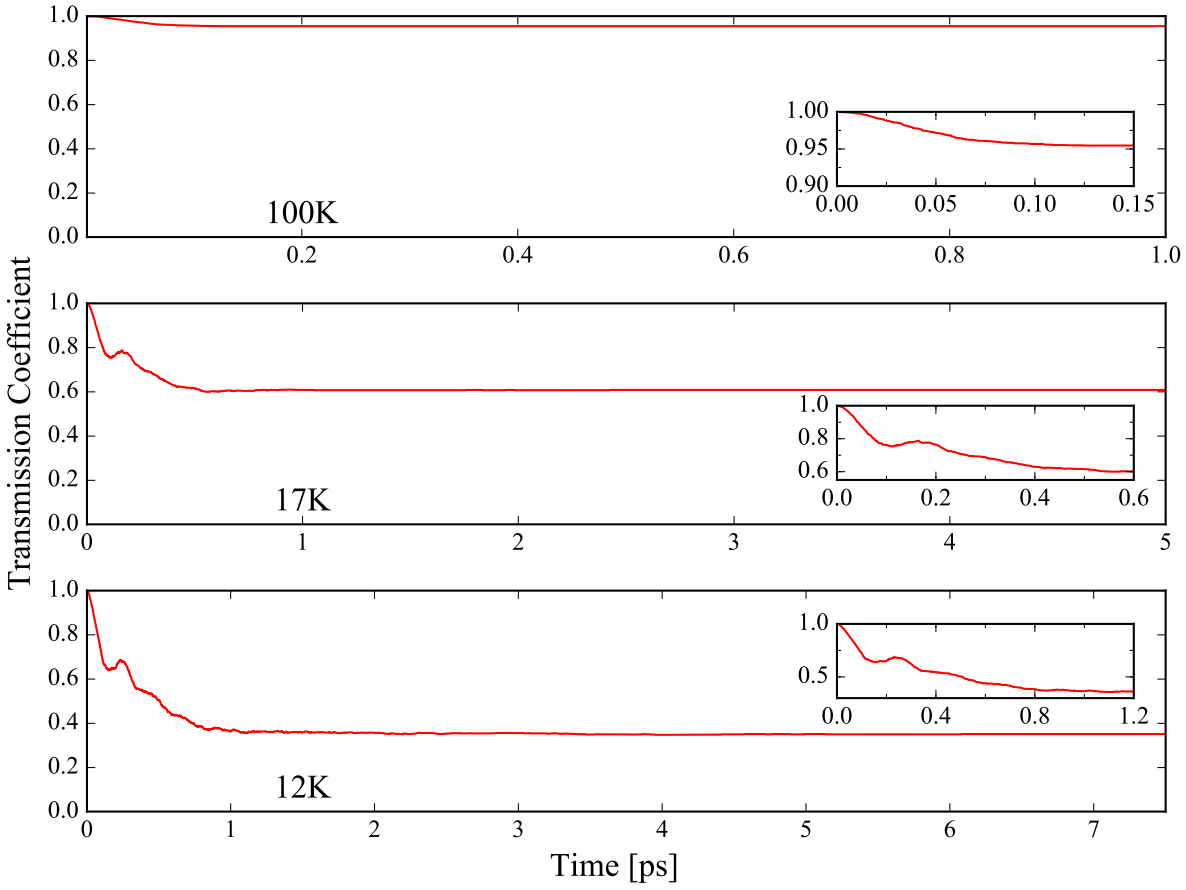

Figure S3. RPMD transmission coefficients for H_2 (red) for temperatures 100K, 17K, and 12K. The y-axis is the same scale for all three graphs, but the x-axis is different due to a longer plateau time at the lower temperatures (17K and 12K).

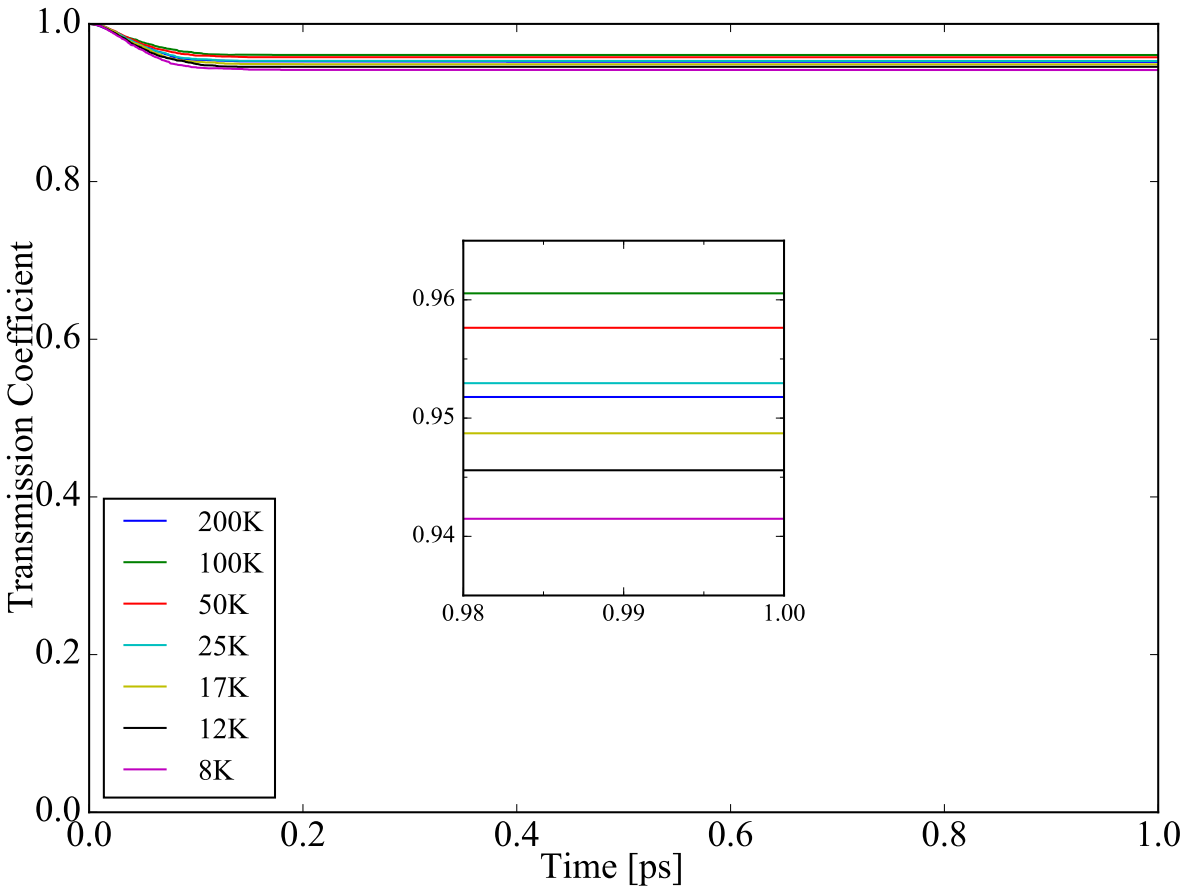

Figure S4. Classical transmission coefficients for all temperatures from 200K to 8K.