

Simulations with importance sampling were carried out over six windows, corresponding to different choices of the umbrella potential, u' . As in previous applications, harmonic forces centered at different values of r_c were used in the present study.¹⁴ The force constants were chosen to be progressively smaller when going from the transition-state region to the products region, reflecting the expected steepness of the energy profile. In addition to the harmonic force, it was found necessary to add an exponential biasing potential to ensure uniform sampling, especially near the transition state. The final choice of the umbrella potential is given