Abstract:
Transition state discovery via application of string methods has been researched on two fronts. The first front involves development of a new string method, named the Searching String method, while the second one aims at estimating transition states from a discretized reaction path. The Searching String method has been benchmarked against a number of previously existing string methods and the Nudged Elastic Band method. The developed methods have led to a reduction in the number of gradient calls required to optimize a transition state, as compared to existing methods. The Searching String method reported here places new beads on a reaction pathway at the midpoint between existing beads, such that the resolution of the path discretization in the region containing the transition state grows exponentially with the number of beads. This approach leads to favorable convergence behavior and generates more accurate estimates of transition states from which convergence to the final transition states occurs more readily. Several techniques for generating improved estimates of transition states from a converged string or nudged elastic band have been developed and benchmarked on 13 chemical test cases. Optimization approaches for string methods, and pitfalls therein, are discussed.

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