Adequate benchmarking of density functionals is a critical part of functional construction and evaluation, given the absence of a method for systematic improvement of functionals. The work presented herein describes limitation of benchmarking on frozen geometries, i.e. molecular geometries optimized using techniques other than the method being evaluated. It is shown that some DFT-predicted reaction barriers are very geometrically dependent, and as such must be optimized with the functional under consideration for adequate benchmarking. In addition, some numerical issues with modern density functionals will be discussed.
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