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AUTOTST: A FRAMEWORK TO PERFORM AUTOMATED TRANSITION STATE THEORY CALCULATIONS

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High fidelity transition state theory (TST) calculations can provide accurate kinetic parameters, but pose some challenges. For example, setting up these calculations is cumbersome and requires initial guesses of reactant, product, and transition state (TS) geometries. Complex reaction mechanisms often include thousands of reactions, so to find them all the TST calculations need to be automated. To tackle this challenge we have developed AutoTST[1], a tool that can perform TST calculations and obtain kinetic parameter automatically. This open-source tool builds on Reaction Mechanism Generator (RMG)[2], the Atomic Simulation Environment (ASE) [3], and RDKit [4]. RMG provides the framework to identify the family of a reaction and the reaction center of a transition state. Using training data and a functional group decision tree, AutoTST provides guesses for interatomic distances at the reaction center, creates a corresponding bounds matrix, and uses RDKit to embed the bounds matrix in 3D. This TS geometry undergoes a series of partial geometry optimizations, using the ASE interface to a variety of quantum calculators, to arrive at a final TS geometry. TS structures are then verified using vibrational mode analysis or intrinsic reaction coordinate calculations. Finally, CanTherm [2] is used to obtain Arrhenius expressions for the reaction of interest. This tool can already be applied to the hydrogen abstraction, intra-molecular hydrogen migration, and disproportion reaction families, with extension to additional gas phase and heterogeneous catalytic reaction families underway.

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