Automating Transition State Searches for Reaction Mechanism Generation

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Accurately describing a reaction system requires understanding details of its mechanism. Such detailed kinetic models can contain over 10,000 unique reactions. Constructing these mechanisms by hand can be a fallible and laborious process, but the rule-based Reaction Mechanism Generator (RMG) can avoid these pitfalls. Published sources are preferentially used for RMGs reactions, with estimation methods deputizing when data are unavailable. Estimates can be improved by applying Transition State Theory. We show how using distance geometry matrices to place reacting atoms in proximity and interpolating between the reactant and product geometries may produce the transition state geometry.