172 - Robust methods for predicting the transition states of chemical reactions: New approaches that focus on key coordinates

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A new method for optimizing transition state and minima structures using redundant internal coordinates is presented. The new method is innovative because it allows the user to select a few key reduced coordinates, whose Hessian components will be accurately computed by finite differencing; the remaining elements of the Hessian are approximated with a quasi-Newton method. Usually the reduced coordinates are the coordinates that are involved in bond breaking/forming. In order to develop this method, several other innovations were made, including ways to (a) select the key reduced coordinates automatically, (b) guess the transition state quickly and efficiently, (c) choose dihedrals so that the "linear angle problem" is avoided, (d) robustly convert redundant internal coordinates to Cartesian coordinates. These, and other technical developments (e.g., new quasi-Newton Hessians, new trust-radius updates), were validated using a database of 7000 initial transition-state guesses for a diverse set of 140 chemical reactions.

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