

Joint CQSE and CASTS Seminar

Weekly Seminar
Nov. 4, 2011 (Friday)

TIME Nov. 4, 14:30 ~ 15:30
TITLE Constrained Multi-Coordinate Driven Method for Locating
Transition States
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Abstract

The multicoordinate driven (MCD) method by Berente and Náray-Szabó [1] can be used to locate high-energy transition states in reactions with large flexible molecules. The direction of the MCD search is defined by a small set of internal coordinates, called driving coordinates. Problems arise when strong coordinates such as covalent bonds are combined with weak ones like dihedral angles in the set of driving coordinates. The weak coordinates tend to pull the search into the direction of the energetically lower lying transition state (like a conformational change) and thereby to mislead the search. Three methods to keep the search on track are proposed: Static limits for the search area, a limited step size and dynamic constraints. The first two methods are implemented via constraining harmonic and anharmonic potentials on the level of the energy-predicting step while the activation of dynamic constraints depends on the strong coordinates. All three methods enable the successful application of the MCD method to reactions where formation of new bonds is accompanied by large conformational changes. The application of a limited search area to keep the search in a computationally feasible area is also discussed. The reversion of the original search direction as the search hits the boundary of computationally non-singular geometries also can be used to prevent the overestimation of the values of the weak coordinates in the transition state.

