Modeling Chemical Reactions in the 21st Century: Picking the Right Method AND the Right Problem*

Rex T. Skodje

Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309 USA
Rex.Skodje@colorado.edu

Theoretical tools for modeling chemical reactions have become quite highly developed and diverse. This confronts us with many choices in tailoring the theoretical description of a reaction to the requirements of specific applications. We shall review several reactions we have recently treated that required different levels of theory: $F+HCl \rightarrow HF+Cl$ (1), $HO_2+HO_2 \rightarrow H_2O_2+O_2$ (2), $CH_2FOH \rightarrow CH_2O+HF$ (3), and $CH_3OH+HO_2 \rightarrow CH_3O+H_2O_2$ (4). We shall emphasize the role of reactive complexes, torsional motion of the collision complex, and the possibility of water photo-catalysis in the discussion. In addition to selecting the appropriate method to model a given reaction, we also need to face the question of determining which reaction in a given mechanism is the most important to investigate. We shall describe some recent advances in global sensitivity analysis for identifying key reactive steps in large mechanisms.

** Collaborative work, in part, with MJ Davis, V Vaida, L Harding, and K Han*

WEDNESDAY

References

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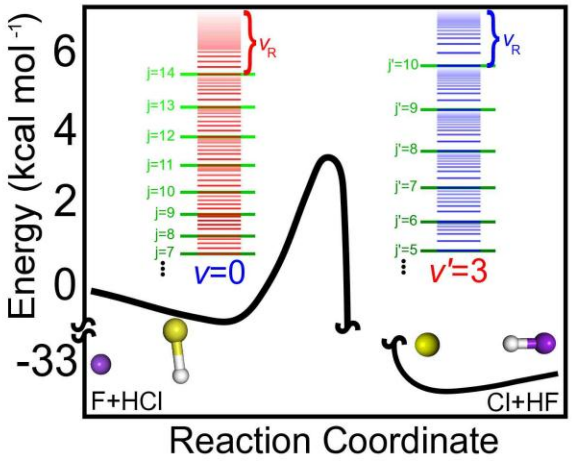
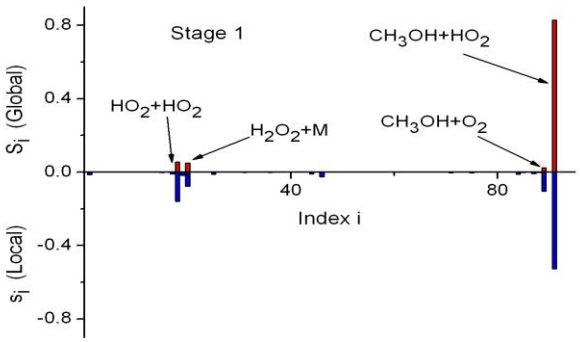


Resonance structure of the F+HCL reaction



Global sensitivity analysis of methanol combustion