Development of specific reaction parameters for SN2 reactions

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The specific reaction parameters (SRP)[1] model was designed to re-optimize the parameters of a semi-empirical QM model (AM1, PM3, …) to high level ab-initio, to get better performance for a particular reaction or class of reactions. We have worked on simplifying and automatizing the basic procedure of developing SRP for SN2 reactions.

Currently, we start from an AM1 model and optimize the parameters over a rigorous sample space (i.e. ±20% of the initial AM1 model) to get a comparable accuracy to *ab initio* MP2 results. We demonstrate that AM1 parameters can be adjusted to rather accurately reproduce MP2 results.

The optimization of semi-empirical parameters consists of the following steps:

- Find the transition structure (TS) at an MP2 level in-vacuo and do the intrinsic reaction coordinates (IRC) scan in both directions.
- Extracting the conformations along the IRC path.
- Run single points calculation by MP2 method and extract relative energies (to the energy of the reactants) and Hessian matrices.
- Fit of the AM1-SRP parameters.
- Final check: IRC, frequency, etc.

Future work would involve the testing of the current procedure on more reactions and the integration of the procedure to the overall software infrastructure of this project.

References

1. Gonzalez-Lafont, A.; Truong, T.; Truhlar, D. G. J. Phys. Chem. 1991, 95, 4618.