Development of an Extrapolation Method for Platinum-Based Molecules

Daniel Süß, Andreas Mauracher, Stefan E. Huber

University of Innsbruck, Institute of Ion Physics and Applied Physics, Technikerstr. 25/3, 6020 Innsbruck, Austria

Platinum-based molecules are among the most leading substances administered in the course of anticancer chemotherapy [1]. For the numerical description of molecular processes involving these molecules (especially in the relevant biomolecular environment) no computationally efficient and accurate standard procedure at the electronic structure level has been established so far. In order to contribute towards this goal, we compare in this contribution various density functionals and extrapolation schemes (similar to Gn methods of Curtiss and co-workers [2, 3]) concerning their performance with respect to geometric and energetic properties of platinum-containing compounds. Our hitherto exploratory study is restricted to a set of molecules for which experimental data of a reasonable accuracy for validation purposes exist. The choice of functionals is based on earlier investigations concerning relative accuracies of different functionals and on the other hand on the application of some typical density functionals (e.g. B3LYP) in applied research. Our small test set for platinum containing molecules is also accompanied by another test set consisting of selected non-metal, organic compounds to monitor the performance of the considered density functionals also concerning the latter test set due to its relevance in the biomolecular setting. In this contribution the key findings such as advantages and disadvantages of the tested methods are presented.

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