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Autobench-RX: A software for automatic reaction barrier calculations

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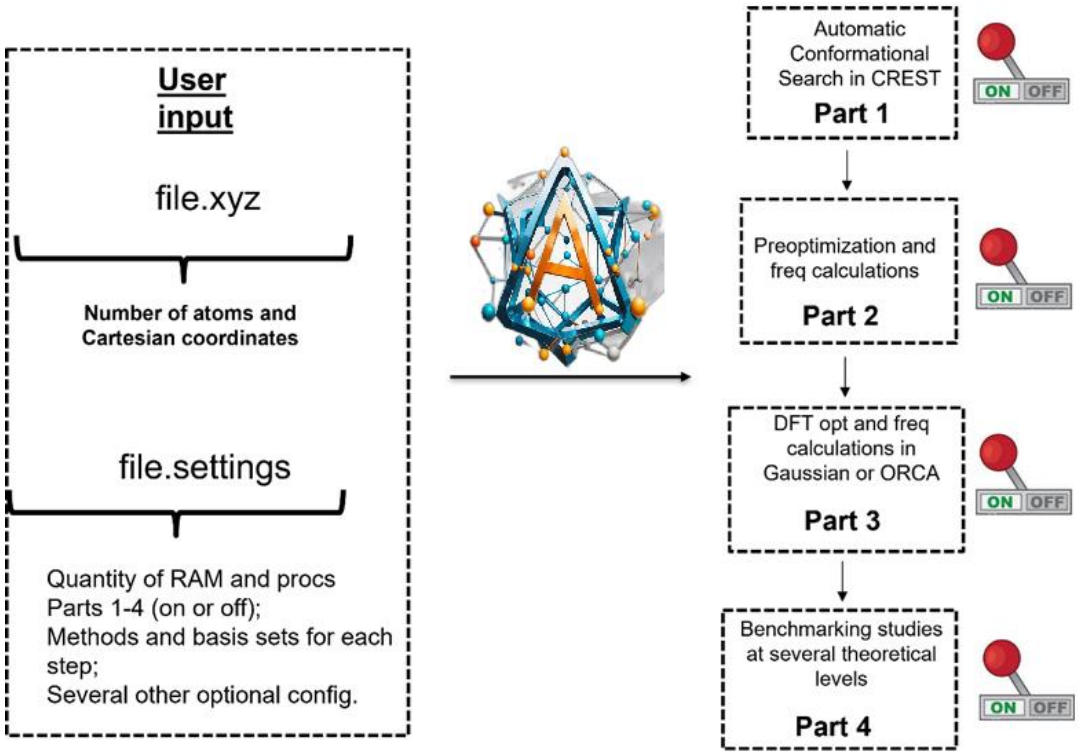
ABSTRACT

This work reports on new software for automatic reaction barrier calculation and benchmarking. This is a new version of Autobench[1] for reaction barrier calculations, coined as Autobench-RX. As its previous version, Autobench-RX workflow consists of four parts (Figure 1): conformational search for transition states, preoptimization, optimization and frequency calculations at a higher level and lastly calculations using several theoretical levels. The software was written to be user friendly and versatile to be used by non-experts in computational chemistry. Any theoretical levels available in either Gaussian 16 or ORCA 5 may be applied in the benchmarking study. The workflow will automatically run conformational search calculations and deal with conformers that converge to the same minimum and those that do not show a single imaginary frequency. At the end of the workflow, the user will have the intrinsic reaction coordinate and Gibbs free energy barriers for several theoretical levels that can be used to compare with experimental data for the reaction of interest.



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