TransRot: a portable and easy-to-use open source software package for simulated annealing Monte Carlo geometry optimization of nanoparticles.

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Preliminary determination of the global minimum geometry of a nanocluster system through the use of an interaction force model prior to *ab initio* calculations is useful in the study of nanoparticles as well as in gas phase nano-solvation studies. To achieve this, our research group has developed a special purpose, open-source software package using our MW-SSA algorithm. TransRot is distributed through GitHub, is written in Java, is machine portable, and is actively supported and maintained. It can be natively installed in all major operating systems (Linux, macOS, and Windows) and is capable of parallel execution of multiple instances on a personal workstation. TransRot is numerically efficient and its behavior is easily controlled through edits to a single short, simple text file. The quasi-ergodicity issue of the original Metropolis-Hastings Monte Carlo algorithm is reduced with the incorporation of a move strategy with randomly magnified step-size and rotational movements ("mag-walking"), as well as a customizable simulated annealing schedule which enhances the probability of escape from local minima. We also present a step-by-step tutorial on how to install and execute Monte Carlo calculations of homogeneous and heterogeneous cluster systems described with OPLS-style models. The code's ability to optimize small water clusters (2 to 8 molecules) described via the TIP3P, TIP4P, and TIP4P/2005 models are compared to the literature. Due to its machine portability, ease of use, and numerical efficiency, TransRot can be also used by an undergraduate or novice graduate student for computational chemistry research and educational purposes.