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

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TransRot GitHub QR Code:

1. Background

Overview: Preliminary determination of the global minimum geometry of a nanocluster system with an interaction force model prior to *ab initio* calculations is useful in nanoparticles and gas-phase nano-solvation studies.

Model: Interaction Potential to assess molecule structures.

$$V = \sum_i \sum_{j>i} \left[A_{ij} exp(-B_{ij} r_{ij}) + \frac{D_{ij}}{r_{ij}^{12}} - \frac{C_{ij}}{r_{ij}^{6}} + \kappa \frac{Q_i Q_j}{r_{ij}} \right]$$

Jorgensen et al. *J. Chem. Phys.* (**1983**)

Challenge: Identifying the global minimum due to the exponentially increasing number of local minima.

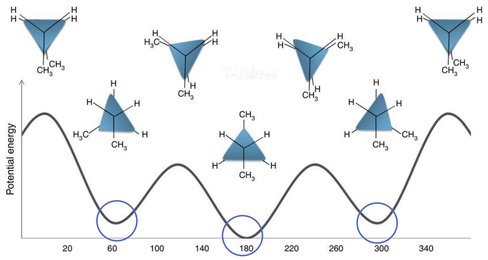


Fig 1. Newman projections and 3 local minima for butane
Khalilian et al. *Educación Química* (**2016**)

Metropolis Monte Carlo: Find lower energy structures via random translational movements.

Generate x'
(Make a trial move)

The Original Metropolis Algorithm:

Translate an atom within a small cube by a random amount

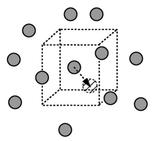


Fig 2. Mechanism of Monte Carlo translational movement
Topper et al. *Reviews in Computational Chemistry* (**2003**)

2. TransRot

Purpose: Our research group has developed a special purpose, open-source Monte Carlo geometry optimization software package using our MW-SSA algorithm.

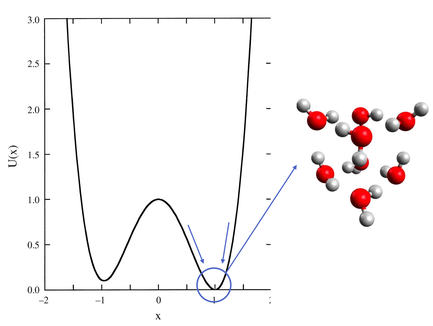


Fig 3. Asymmetric double-well potential
Topper et al. *Reviews in Computational Chemistry* (**2003**)

Operating systems: TransRot is natively installed in Linux, macOS, and Windows and is capable of parallel execution of multiple instances on a personal workstation.

MW-SSA Algorithm: Our MW-SSA algorithm improved the quasi-ergodicity issue of the original Metropolis Algorithm by introducing

1) **Varying step-size:** randomly magnified step-size rotational movements ("mag-walking").
2) **Customizable annealing:** system is cooled, reheated, and re-cooled to avoid premature trapping.

3. Test TransRot

Method: The code's ability to optimize small water clusters (2 to 8 molecules) described via the TIP3P and TIP4P models were compared to the literature.

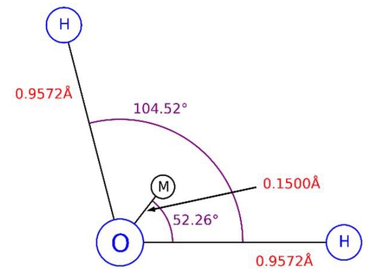


Fig 4. TIP4P water model diagram

Table 1. TIP4P Global Minimum Energy Comparison

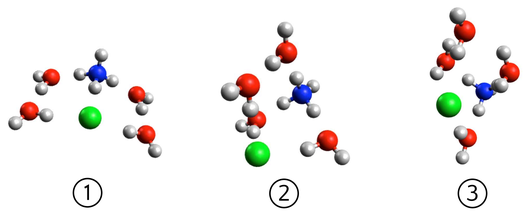
N	*Wales (kJ/mol)	TransRot (kJ/mol)	Difference (kJ/mol)
2	-26.088	-26.087	**0.001**
3	-69.994	-69.993	**0.001**
4	-116.590	-116.588	**0.002**
5	-152.109	-152.106	**0.003**
6	-197.781	-197.777	**0.004**
7	-243.572	-243.568	**0.004**
8	-305.518	-305.513	**0.005**

*Wales et al. *Chem. Phys. Lett* (**1988**)

4. TransRot in Practice

Our Study: We study the formation of ammonium chloride (NH_4Cl) nano-solvated in water clusters ($N{\cdot}H_2O$)

3 minima were found for N=4

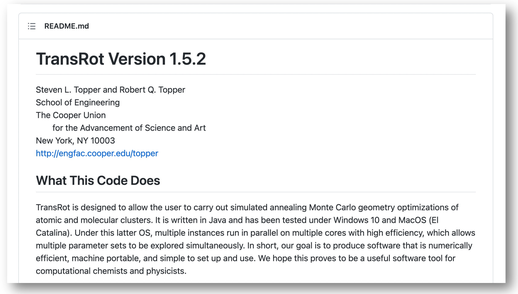


ΔE_{12} = 9.4 kJ/mol
ΔE_{23} = 8.1 kJ/mol

5. Future Work

Development: TransRot is fully documented and maintained by the Topper research group. We plan to add:

1) **More force fields:** Lennard-Jones or Buckingham potentials
2) **More parameters**: Force field parameters for molecules and elements.


README.md

TransRot Version 1.5.2

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What This Code Does

TransRot is designed to allow the user to carry out simulated annealing Monte Carlo geometry optimizations of atomic and molecular clusters. It is written in Java and has been tested under Windows 10 and MacOS (El Catalina). Under this latter OS, multiple instances run in parallel on multiple cores with high efficiency, which allows multiple parameter sets to be explored simultaneously. In short, our goal is to produce software that is numerically efficient, machine portable, and simple to set up and use. We hope this proves to be a useful software tool for computational chemists and physicists.

Fig 5. TransRot GitHub repository

6. Conclusion

Due to its (1) machine portability, (2) ease of use, and (3) numerical efficiency, TransRot can be also used by an undergraduate or novice graduate student for computational chemistry research and educational purposes.

Acknowledgements

Steven L. Topper is the developer of TransRot; Robert Q. Topper is the projector director of TransRot; Sangjoon Lee has conducted case studies of TIP4P/NH_4Cl($N{\cdot}H_2O$) and designed this poster. Elliot Topper helped with Fig 4.