tesliper: a theoretical spectroscopist's little helper

Michał M. Więcław[1][¶]

1 Institute of Organic Chemistry, Polish Academy of Sciences ¶ Corresponding author

Summary

`tesliper` is a software package for the bulk processing of Gaussian (quantum chemistry calculations software) output files regarding conformational searches and spectra simulations. Simulation of a molecule's optical spectra usually requires structure optimization and calculation of the electronic properties of multiple conformers of the studied molecule. Gaussian (Frisch et al., 2016) is one of the most commonly used software packages to perform such calculations and `tesliper` was created to aid the handling and analysis of these calculations' outputs.

It allows for easy exclusion of conformers that are not suitable for further analysis: erroneous, not optimized, of higher energy or lower contribution than a desired threshold. It also implements a geometry comparison feature: an RMSD sieve, enabling the filtering out of similar structures. A theoretical IR, VCD, UV, ECD, Raman, and ROA spectra may be calculated for individual conformers or as a population-weighted average. Offering a graphical user interface and Python API, it is easily accessible by the users' preferred method of interaction with the computer: visual or textual.

Statement of Need

Simulation of optical spectra of organic compounds has become a routine task for chemical analysts. For example, it is a necessary step in one of the increasingly popular methods of establishing a compound's absolute configuration through comparison of recorded and simulated circular dichroism spectra. However, the process of obtaining a simulated spectrum may be cumbersome, as it usually involves analyzing a large number of potentially stable conformers of the studied molecule.

Several software packages capable of simulating a spectrum from Gaussian calculations are already available, e.g. SpecDis (Bruhn et al., 2013), CDspecTech (Covington & Polavarapu, 2017), ComputeVOA (Debie et al., 2010), ChemCraft (*Chemcraft - Graphical Software for Visualization of Quantum Chemistry Computations*, n.d.), or GaussView (Dennington et al., 2016). However, each of these programs has some severe limitations, for example they are not freely available (ComputeVOA, ChemCraft, GaussView) or cannot simulate certain types of spectra (SpecDis, ComputeVOA, ChemCraft). Other packages lack important features, like comparison of conformers' geometry (SpecDis, CDspecTech, GaussView) or population-based spectra averaging (ComputeVOA, ChemCraft, GaussView).

Even with adoption of one or more of the software packages mentioned above, the process is often suboptimal, incomplete, or unable to be done in an automated fashion. Many research groups tackle this problem with home-brewed scripting solutions that are usually not easily adjusted or extended, or with manual work, which may be extremely time-consuming. There is a clear need for a simple interface to automate tedious parts of the typical spectra simulation workflow. `tesliper` aims to satisfy this need.

Acknowledgements

References

Bruhn, T., Schaumlöffel, A., Hemberger, Y., & Bringmann, G. (2013). SpecDis: Quantifying the comparison of calculated and experimental electronic circular dichroism spectra. *Chirality*, *25*(4), 243–249. https://doi.org/10.1002/chir.22138

Chemcraft - graphical software for visualization of quantum chemistry computations. (n.d.). https://www.chemcraftprog.com

Covington, C. L., & Polavarapu, P. L. (2017). CDSpecTech: A single software suite for multiple chiroptical spectroscopic analyses. *Chirality*, *29*(5), 178–192. https://doi.org/10.1002/chir.22691

Debie, E., L. A. Nafie, P. B. nd, & Dukor, R. K. (2010). *ComputeVOA*. BioTools Inc. https://biotools.us/software-2

Dennington, R., Keith, T. A., & Millam, J. M. (2016). *GaussView version 6*.

Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A. V., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., … Fox, D. J. (2016). *Gaussian 16*.