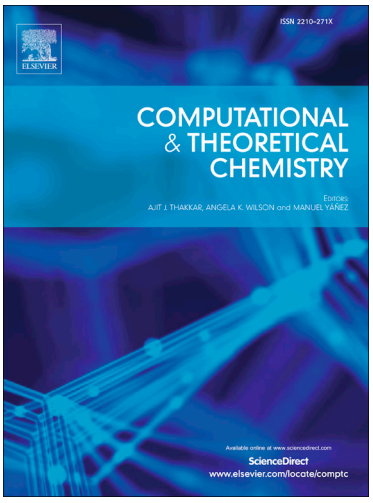

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PII: S2210-271X(18)30003-3
DOI: https://doi.org/10.1016/j.comptc.2018.01.003
Reference: COMPTC 2697

To appear in: *Computational & Theoretical Chemistry*

Received Date: 14 November 2017
Revised Date: 1 January 2018
Accepted Date: 1 January 2018

Please cite this article as: H. Jang, N. Joon Kim, J. Heo, Benchmarking Study on Time-Dependent Density Functional Theory Calculations of Electronic Circular Dichroism for Gas-Phase Molecules, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.01.003

Benchmarking Study on Time-Dependent Density Functional Theory Calculations of Electronic Circular Dichroism for Gas-Phase Molecules

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Abstract

Time-dependent density functional (TDDFT) theory has become a popular method to calculate electronic excited states. The electronic circular dichroism (ECD) spectra of chiral molecules can be computed by TDDFT to resolve their absolute configurations. In this work, we evaluated the performance of TDDFT to calculate ECD of three chiral molecules whose vibronic CD spectra in a supersonic jet were recently reported. We tested seven different functionals (PBEPBE, PBE1PBE, B3LYP, mPW1PW91, M06-2X, CAM-B3LYP, and ωB97X-D) with different levels of the Pople basis set to predict the rotatory strengths of both vertical and adiabatic excitations of the chiral molecules. The 6-311++G(d,p) basis set is appropriate for the ECD calculation, and the augmentation of the diffuse function improves the quality of basis set in calculating the rotatory strength. The simulations of vibronic CD spectra under the adiabatic Hessian scheme in Cartesian coordinates have been feasible only with the M06-2X, CAM-B3LYP, and ωB97X-D functionals. The rotatory strength signs for