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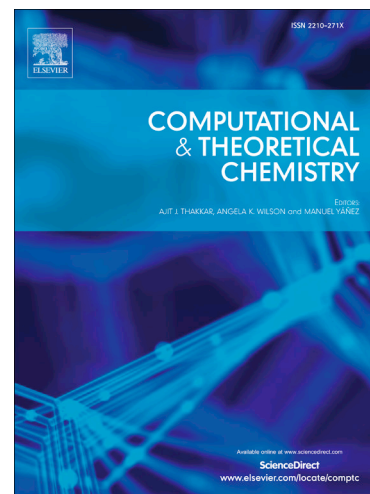
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Benchmarking Study on Time-Dependent Density Functional Theory Calculations of Electronic Circular Dichroism for Gas-Phase Molecules

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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 ω B97X-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 ω B97X-D functionals. The rotatory strength signs for

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