

Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane

Autorzy

Vincenzo Barone

Małgorzata Biczysko

Julien Bloino

Cristina Puzzarini

Rok wydania

2014

Czasopismo

Journal of Chemical Physics

Numer woluminu

141

Strony

034107/1-034107/17

DOI

10.1063/1.4887357

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Oxirane derivatives are the most used benchmarks for chiroptical spectroscopies in view of their small size and relative rigidity. The molecular structure, vibrational harmonic and anharmonic frequencies, and infrared intensities of the ground electronic states are analyzed in this paper. Equilibrium structure and harmonic force fields have been evaluated by means of high-level quantum-chemical calculations at the coupled-cluster level including single and double excitations together with a perturbative treatment of triples (CCSD(T)). Extrapolation to the complete basis-set limit as well as core-correlation effects have also been taken into account. Anharmonic contributions have been computed at the CCSD(T)/cc-pVTZ level for trans-2,3-dideuterooxirane. These data can serve as references to evaluate the accuracy of less expensive computational approaches rooted in the density functional theory (DFT). The latter have been used within hybrid CC/DFT approaches, which have been applied to simulate fully anharmonic infrared (IR) spectra. Finally, the best theoretical estimates of the equilibrium structures and vibrational wavenumbers are compared to the most accurate experimental data and show in all cases very good agreement, i.e., within 0.001 Å, 0.1 deg, 10 cm⁻¹, and 0.5 km mol⁻¹, for bond lengths, angles, wavenumbers, and IR intensities, respectively.

Słowa kluczowe

Coupled-cluster methods, Density functional theory, Correlation energy, Correlation-consistent basis sets, Hybrid functionals, Computational models, Molecular structure, Infrared spectroscopy, Gas phase, Chemical compounds

Adres publiczny

<http://dx.doi.org/10.1063/1.4887357>

<https://www.aip.org/>

Plik został wygenerowany dnia 2026-08-23 22:06:07

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/oX6lEXp>.