

Molecular Structure and Spectroscopic Signatures of Acrolein: Theory Meets Experiment

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Streszczenie

A comprehensive study of the molecular structure and IR spectrum of *cis* and *trans* acrolein has been performed by an integrated computational approach coupling methods rooted in the coupled-cluster ansatz and the density functional theory. From the one side, DFT anharmonic force fields allow us to determine very reliable semi-experimental structures for both isomers, which are in remarkable agreement with the geometries issuing from CCSD(T) computations accounting for the extrapolation to the complete basis set and core correlation. The same kind of coupled-cluster computations provide dipole moment, relative energies, and interconversion barrier in remarkable agreement with experiments. Finally, harmonic CCSD(T) results coupled to DFT evaluation of mechanical and electrical anharmonicity allow us, in the framework of second-order perturbative vibrational theory, to confirm most of the experimental assignments of IR spectra, and to suggest some additional interpretations for congested regions including fundamental bands together with overtones and combination bands.

Słowa kluczowe

Energy, Equilibrium, Molecular mechanics, Molecular structure

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<https://www.acs.org/content/acs/en.html>