

Spectroscopic properties of a strongly anharmonic Mannich base N-oxide.

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Car-Parrinello molecular dynamics simulations in vacuum and in the solid state are performed on a strongly anharmonic system, namely, 2-(N-diethylamino-N-oxymethyl)-4,6-dichlorophenol, to investigate its molecular and spectroscopic properties. The investigated compound contains two slightly different molecules in the crystal cell with very short intramolecular hydrogen bonds (of 2.400 and 2.423 Å), as determined previously by neutron diffraction. The vibrational properties of the compound are studied on the basis of standard approaches, that is, Fourier transformation of the autocorrelation functions of the atomic velocities and dipole moments. Then, the trajectory obtained from ab initio molecular dynamics is sampled and the obtained snapshots are used to solve the vibrational Schrödinger equations and to calculate the O-H stretching envelope as a superposition of the 0→1 transition. Using an envelope method, the a posteriori quantum effects are included in the O-H stretching. In addition, NMR spectra are calculated also using the obtained snapshots. One- and two-dimensional potentials of mean force (1D and 2D pmf) are derived to explain the details of the proton dynamics. The computational results are supported by NMR experimental data. In addition, the calculated results are compared with previously published X-ray, neutron diffraction, and spectroscopic descriptions. A detailed analysis of the bridged proton's dynamics is thus obtained. The application of 1D and 2D pmf in a system with a strong bridged-proton delocalization is also demonstrated.

Słowa kluczowe

Enharmonic systems, Intramolecular hydrogen bonds, Molecular dynamics, NMR spectroscopy, Solid-state studies

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