Accurate spectroscopic characterization of the HOC(O)O radical: A route toward its experimental identification

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Streszczenie

A set of accurate spectroscopic parameters for the detection of the atmospherically important HOC(O)O radical has been obtained by means of state-of-the-art *ab initio* computations. These include advanced coupled cluster treatments, involving both standard and explicitly correlated approaches, to correctly account for basis set incompleteness and core-valence effects. Geometric parameters for the $\tilde{X}^2A'$ and $\tilde{A}^2A''$ states and, for the ground state only, vibrationally corrected rotational constants including quartic and sextic centrifugal distortion terms are reported. The infrared spectrum of the $\tilde{X}^2A'$ state has been simulated in the 4000-400 cm^{-1} wavenumber interval with an approach based on second order vibrational perturbation theory that allows accounting for anharmonic effects in both energies and intensities. Finally, the vibronic spectrum for the $\tilde{A} \leftarrow \tilde{X}$ transition has been calculated at three different temperatures in the 9000-3000 cm^{-1} energy range with a time-independent technique based on the Franck-Condon approximation.

Słowa kluczowe

Coupled-cluster methods, Correlation-consistent basis sets, Perturbation theory, Rotational spectra, Franck Condon factors, Chemical elements, Infrared spectroscopy, Centrifugal distortion, Vibronic transitions, Chemical compounds

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