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Vibrational spectroscopy, Ab Initio calculations and Frontier Orbital analysis
of 4,5,6,8,9-pentachloropyrimido-[1,2-a][1,8]naphthyridin-10-one

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ABSTRACT

In this work we present a study of the vibrational spectra of 4,5,6,8,9-pentachloropyrimido-[1,2-a][1,8]naphthyridin-10-one, $C_{11}H_2Cl_5N_3O$, a substance belonging to the important pharmacological class of 1,8-naphthyridine derivatives. The Fourier transform infrared and the Fourier transform Raman spectra of the crystal were recorded at room temperature in the regions 400 cm^{-1} to 4000 cm^{-1} and 50 cm^{-1} to 4000 cm^{-1} , respectively. Vibrational wavenumbers were predicted using density functional theory calculations with the B3LYP functional on 6-31G(d,p) and 6-311++G(d,p) basis sets. The descriptions of the normal modes were made after calculating the potential energy distribution. Additionally, potential reaction sites were evaluated through Mulliken population and Frontier Orbital analysis.

Keywords: Raman scattering; IR spectroscopy; DFT; $C_{11}H_2Cl_5N_3O$ crystal

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