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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

C.E.S. Nogueira[a*], P.E.S. Caselli[b] , P.T.C. Freire[b], A.M.R. Teixeira[a], I.M.M. Oliveira[a], R.R.F. Bento[c], J.L.B. Faria[c], G.O.M. Gusmão[d,b], L.E. Silva[e]

[a] Departamento de Física, Universidade Regional do Cariri, 63010-970, Brazil

[b] Departamento de Física, Universidade Federal do Ceará, 60455-760, Brazil

[c] Departamento de Física, Universidade Federal de Mato Grosso, 78060-900, Brazil

[d] Universidade Estadual do Piauí, Teresina-PI, 64002-150, Brazil

[e] Universidade Federal do Paraná, Setor Litoral - Matinhos, 83260-000, Brazil

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

* Corresponding author. Phone: 55-88-9985 6159, Fax: 55-88-3102 1294.

E-mail address: carlosemidio@ymail.com (C.E.S. Nogueira).