



Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

Volume 123, 5 April 2014, Pages 89-97

FT-IR, FT-Raman spectra and other molecular properties of 2,4-dichlorobenzonitrile: A interpretation by a DFT study

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<https://doi.org/10.1016/j.saa.2013.12.052> 

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Abstract

FT-IR and FT-Raman spectra of 2,4-dichlorobenzonitrile at room temperature have been recorded in the regions $200\text{--}3500\text{cm}^{-1}$ and $0\text{--}3400\text{cm}^{-1}$, respectively. The observed vibrational bands were analyzed and assigned to different normal modes of the molecule according to the Wilson's notation. Density functional calculations were performed to support our frequency assignments. Specific scale equations deduced from the benzene molecule were employed to improve the calculated values. For the majority of the normal modes, the deviations between the corresponding experimental and scaled theoretical wavenumbers are located in the expected range. A correct characterization of each normal mode is of vital importance in the assignment of the observed bands, and the same has been successfully done by the aid of Potential Energy Distributions (PEDs) calculated separately for each normal mode of 2,4-dichlorobenzonitrile. The molecular structure was optimized and several thermodynamic parameters were determined. HOMO and LUMO orbital energy analysis were carried out.

Graphical abstract