Characterization (FT-Raman, FT-II Spectra) of 3.5-Dimethoxybenzaldehyde C₉H₁₀O₃ and Compared with Density Functional Theory (DFT)

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ABSTRACT

The FT-IR and FT-Raman spectra of 3.5- dimethoxybenzaldehyde C9H10O3 molecule have been recorded in the range of 4000–400 cm⁻¹ and 3500–50 cm⁻¹ respectively. The molecular geometry and vibrational frequencies in the ground state are calculated using the DFT/B3LYP method with 6-311G++(d,p) basis sets and assuming CS symmetry. The computed values of frequencies are scaled using a suitable scale factor to yield good coherence with the observed values.

Keywords: FT-Raman, FT-IR, DFT, 3.5-dimethoxybenzaldehyde

Introduction

This work is a part of a systematic study about, the molecular conformation and the spectroscopic behavior of the methylbenzene in the solid state. One of the interests of these materials lies in the fact that they allow to study in details the influence of the molecular environment to perturb their symmetry and in particular the consequences on the spectroscopic properties.

Experimental/TheoreticalStudy

FT-IR SPECTROSCOPY

The FT-IR spectra (500-3500 cm⁻¹ region) were recorded on the Jasco (FT/IR-6300) spectrometer at room temperature with with 4.0 cm⁻¹ resolution. Each band is characterized by its value of v at the maximum of absorption.

RAMAN SPECTROSCOPY

The Raman spectra were made with μ -Raman Bruker Senterra in the range of 3500 to 100 cm⁻¹, equipped with a 100 mW laser source operated at λ =785 nm,and aperture setting about 20 ×1000 μ m.

QUANTUM CHEMICAL CALCULATIONS

The geometry of bromodurene was fully optimised using the DFT/B3LYP [1] method with 6-311G++(d,p), which has proven to give a very ground state geometry.

Results and Discussion

From an overall point of view, three frequency domainscan be distinguished: 16 frequency modes below 600 cm⁻¹, 34 between 600 and 1700 cm⁻¹, and 10 frequency modes above 1700 cm⁻¹ Among the 60 modes of vibration, 41 modes are active in FT-IR and Raman, 6 are active only in Raman, 10 are



active only in IR and the other 3 modes are not active. In the Raman spectrum, the extremely intense line at 991vs cm⁻¹ calculated at 1002 cm⁻¹ from DFT is generated by the phenyl ring vibrations (Breathing ring). In the IR spectrum two strong bands at 1163vs and 1200vs cm⁻¹ arise from the mixed (ip C–H) in- plane bending vibrations.

The agreement between the calculated and experimental frequencies is very good: always better than 97% for the observed skeletal vibrations. The calculations overestimate the methyl frequencies by 7%, and experiment shows only broad features for these excitations.

Conclusion

The vibrational frequencies, infrared intensities, and the Raman activities of the compound are calculated by DFT/B3LYP and compared with experimental data. The small difference between calculated and experimental wave numbers could be a consequence of the presence of vibrations of the intermolecular interactions in the crystals that were completelymissing in the DFT calculation.

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References

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