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FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular conformational analysis of 2,5-di-tert-butyl-hydroquinone

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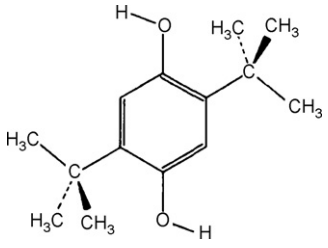
ABSTRACT

The purpose of finding conformer among six different possible conformers of 2,5-di-tert-butyl-hydroquinone (DTBHQ), its equilibrium geometry and harmonic wavenumbers were calculated by the B3LYP/6-31G(d,p) method. The infrared and Raman spectra of DTBHQ were recorded in the region 400–4000 cm^{-1} and 50–3500 cm^{-1}, respectively. In addition, the IR spectra in CCl_4 at various concentrations of DTBHQ are also recorded. The computed vibrational wavenumbers were compared with the IR and Raman experimental data. Computational calculations at B3LYP level with two different basis sets 6-31G(d,p) and 6-311++G(d,p) are also employed in the study of the possible conformer of DTBHQ. The complete assignments were performed on the basis of the potential energy distribution (PED) of the vibrational modes, calculated using VEDA 4 program. The general agreement between the observed and calculated frequencies was established.

1. Introduction

Free radicals can damage the cells and may play a role in heart disease, cancer and other diseases. Antioxidants are substances that may protect cells against the effects of free radicals. It is known that quinone derivatives especially hydroquinone and its certain derivatives are capable of inhibiting free-radical fragmentation reactions which play an essential role in the damage of biologically important molecules [1–3]. 2,5-Di-tert-butyl-hydroquinone (DTBHQ), an important derivative of hydroquinones, is used as an inhibitor, antioxidant and stabilizer. It is useful as an antioxidant for rubber products, a stabilizer and an anti-skinning agent in paints. There are several investigations about antioxidant property of DTBHQ [4–6].



Nowadays FT-IR and FT-Raman spectroscopy combined with quantum chemical computations is used as an effective tool in the vibrational analysis of drug molecules [7], biological compounds [8] and natural products [9], since the vibrational spectra and the computed results can help unambiguous identification of vibrational modes as well as the bonding and structural features of complex organic molecular systems.

Magnetic properties of DTBHQ were studied using theoretical and experimental EPR technique by our group recently [10]. To the best of our knowledge, neither quantum chemical calculations, nor the vibrational spectra of DTBHQ have been reported, as yet. The aim of the present work is the conformational analysis understanding of the structural information, and the full assignment of the vibrational spectra (harmonic wavenumbers, and relative intensities for Raman and IR spectra) of DTBHQ by means of density functional theory (DFT) studies. The calculated vibrational frequencies are compared with those observed experimentally.

2. Experimental

The powder form of DTBHQ was purchased from Merck. FT-IR spectrum of powder DTBHQ recorded in the range 4000–400 cm^{-1} on Bruker IFS 66/S with PIKE Gladi ATR (Diamond) spectrometer at room temperature with 2 cm^{-1} resolution. The FT-IR solution spectra in CCl_4 at various concentrations of DTBHQ also recorded in the range 400–4000 cm^{-1} in the same instrument. The FT-Raman

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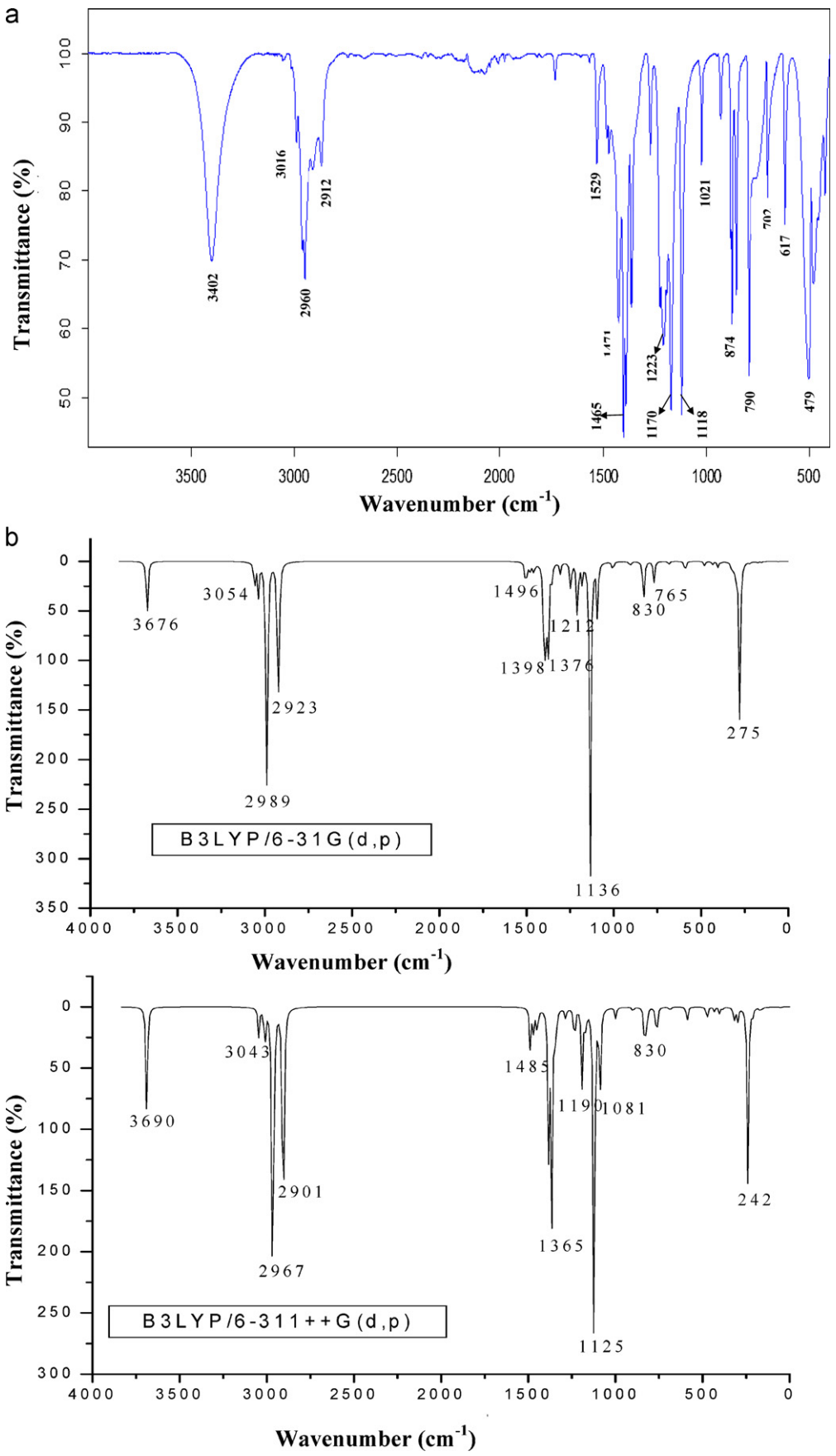

Fig. 1. (a) Experimental (solid phase) FT-IR spectrum of DTBHQ. (b) Theoretical FT-IR spectra of DTBHQ.