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# Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone

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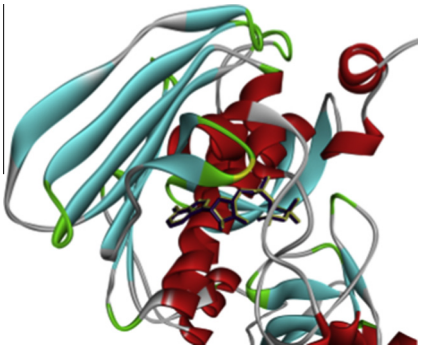
## HIGHLIGHTS

- IR, Raman spectra and NBO analysis were reported.
- The wavenumbers are calculated theoretically using Gaussian09 software.
- Molecular docking studies were reported.
- The geometrical parameters are in agreement with XRD data.

## GRAPHICAL ABSTRACT



## ARTICLE INFO

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## ABSTRACT

FT-IR and FT-Raman spectra of 10,10-Dimethylanthrone were recorded and analyzed. The vibrational wavenumbers were computed using DFT quantum chemical calculations. The data obtained from wavenumber calculations are used to assign vibrational bands obtained experimentally. In its most stable form, the title compound maintains $C_{2v}$ symmetry as determined by XRD results, where both methyl groups are staggered with respect to the corresponding $C_{23}$—$C_{24}$ and $C_{23}$—$C_{28}$ bonds. The geometrical parameters (B3LYP/6-311++G(d,p)(5D,7F)) of the title compound are in agreement with the XRD results. The calculated HOMO and LUMO energies allow the calculations of atomic and molecular properties and they also showed that charge transfer occurs in the molecule. A detailed molecular picture of the title compound and its interactions were obtained from NBO analysis. As seen from the MEP map, negative potential regions are localized over the carbonyl group and are possible sites for electrophilic attack. The title compound, 10,10-Dimethylanthrone forms a stable complex with human topoisomerase-II as is evident from the ligand-receptor interactions and show appreciable antineoplastic activity.



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## Introduction

Anthracene is a material producing electroluminescence and along with its derivatives have still been attracting the attention from the view point of applications and basic science [1]. Anthracene derivatives, which are tricyclic aromatic compounds, are very significant building blocks for the synthesis of dyes and pigments [2,3], pharmaceuticals [4,5], agrochemicals [6], light emitting devices [7] and additives of paper making [8]. They are also potentially useful as significant insecticides, since they are postulated as the chemicals that give teak their resistance to insect and fungal attacks. Structural properties and potential applications were reported for different anthracene derivatives such as anthracyclins, anthraquinones and anthrones. Anthracycline was one of the widely studied drugs owing to its notably clinical efficacy against a variety of human cancers [9]. Moreover, Shamsipur et al. [10] reported the quantitative structure property relationship study of acidity constants of some anthraquinone derivatives using multiple linear regression and partial least squared procedures. Anthrone and related phenols in particular exhibit a solvent-dependent high-diene reactivity in Diels–Alder reactions. Anthrone (9-Hydroxyanthracene) is used as a popular cellulose assay and in the colorometric determination of carbohydrates [11]. Zagotto et al. [12] reported 1,4-anthracene-9,10-dione derivatives as potential anticancer agents. The crystal structures of anthrone [13] and some of its derivatives, such as 10-bromoanthrone [14], 9,10-dimethylanthracene [15], benzylideneanthrone at 193 K [16], 10-(2-methylbenzylidene) anthrone [17], 10-(3,4-dimethoxybenzylidene) anthrone [18] and 10-(4-hydroxy-3-nitrobenzylidene) anthrone [19] have been reported. In addition, vibrational studies on a few anthracene and anthrone derivatives can be found in the literature [20,21]. Chandran et al. [20] reported the vibrational spectroscopic and computational study of (E)-4-((anthracen-9-ylmethylene)amino)-N-carbamimidoylbenzene sulfonamide, an anthracene derivative. The spectroscopic studies of the phenylanthracene-9,10-dione derivative by ab initio HF and density functional methods has been also reported [21]. In the present study, the structural and conformational properties as well as the vibrational infrared and Raman spectra of 10,10-Dimethylanthrone (chemical name:10,10-dimethyl-10H-anthracen-9-one), which is considered is an important intermediate for the preparation of melitracen hydrochloride, are presented.

## Experimental

The title compound was obtained as a gift sample from R.L. Fine Chem., Bangalore, India. X-ray quality crystals were obtained by slow evaporation from methanol solution. The FT-IR spectrum (Fig. 1) was recorded using KBr pellets on a DR/Jasco FT-IR 6300 spectrometer. The FT-Raman spectrum (Fig. 2) was obtained on a Bruker RFS 100/s, Germany. For the excitation laser source of the Raman spectrum, the emission of Nd:YAG laser with an excitation wavelength of 1064 nm and maximal power of 10 mW was used. Measurement was carried out on a solid sample.

## Computational details

For meeting the requirements of both accuracy and computing economy, theoretical methods and basis sets should be carefully considered. Density functional theory has been proven to be extremely useful in treating the electronic structure of the organic molecules. Gaussian09 program [22] was used to carry out the DFT calculations with Becke's three parameter hybrid model and the Lee–Yang–Parr correlation functional (B3LYP) method. The basis set 6-311++G(d,p)(5D,7F), which is an effective level with

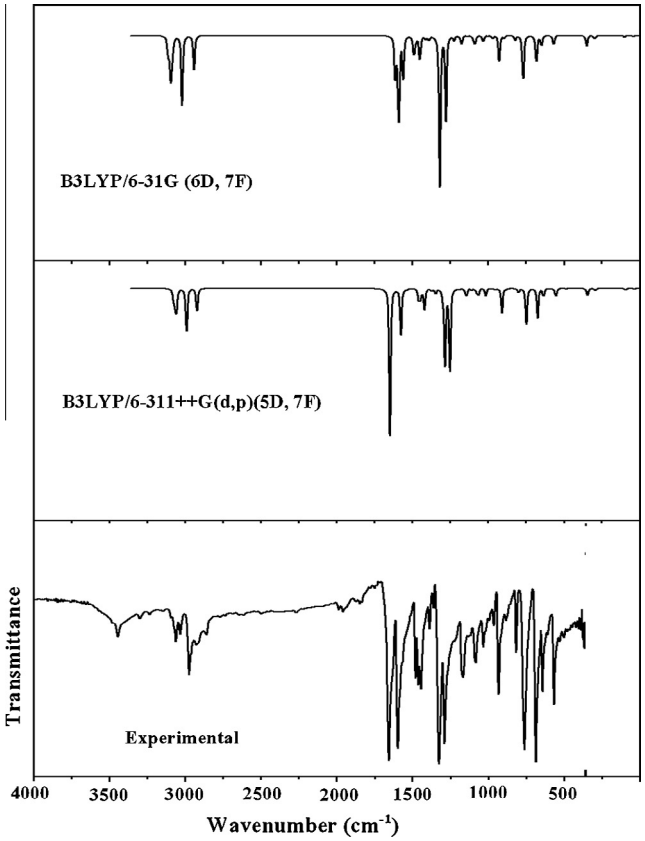


**Fig. 1.** FT-IR spectrum of 10,10-Dimethylanthrone.

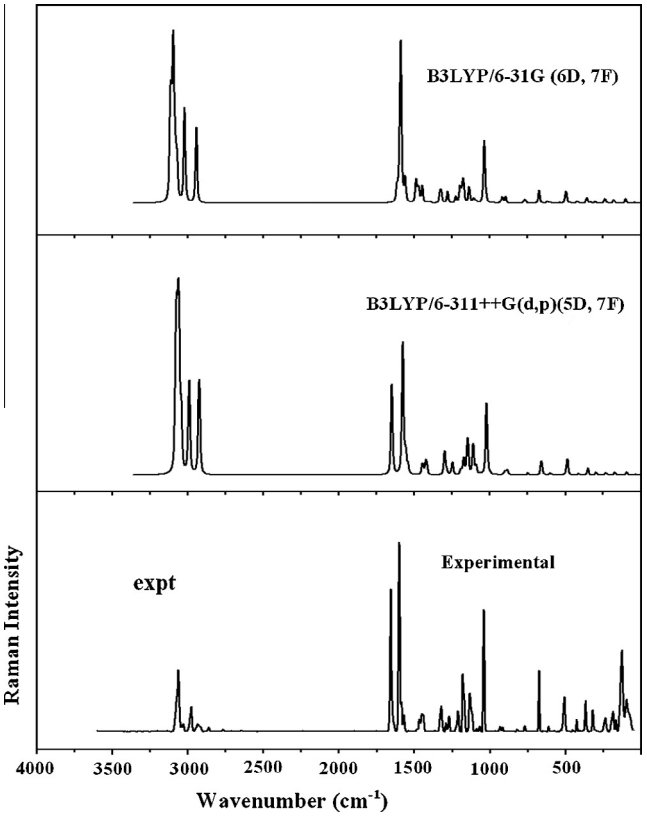


**Fig. 2.** FT-Raman spectrum of 10,10-Dimethylanthrone.