

Antibacterial Property of Essential Oil and its vibrational analysis

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Abstract: In recent years there has been an increasing interest in the use of natural substances, and some questions concerning the safety of synthetic compounds have encouraged more detailed studies of plant resources. Essential oils, odorous and volatile products of plant secondary metabolism, have a wide application in folk medicine, food flavoring and preservation as well as in fragrance industries. In our present work with the vibrational spectroscopy of quantum chemical calculations of Eugenol, Geraniol have been carried out. The compounds are responsible for most of the characteristic aroma. DFT analysis is performed before and after application of clove oil on *Aspergillus* fungi. Vibrational analysis on Eugenol (4-allyl-2-methoxyphenol) is also carried out. The fluorescent property of the material was also discussed.

Key words: Essential oils, Antibacterial activity, Antifungal activity, Eugenol (4-allyl-2-methoxyphenol)

I. Introduction:

The antimicrobial properties of essential oils have been known for many centuries. In recent years (1987-2001) a large number of essential oils and their constituents have been investigated for their antimicrobial properties against some bacteria and fungi in more than 500 reports. (1-5). This paper gives an overview on the susceptibility of human and food-borne bacteria and fungi towards different essential oils and their constituents. (6-8). This work deals with the vibrational spectroscopy of Eugenol by means of quantum chemical calculations. The mid and far FTIR and FT-Raman spectra were measured in the condensed state. The compound Eugenol (4-allyl-2-methoxyphenol) is responsible for most of the characteristic aroma of cloves. DFT analysis is performed before and after application of clove oil on *Aspergillus* fungi. Vibrational analysis on 4-allyl-2-methoxyphenol is also carried out. The fluorescent property of the material was also discussed. Clove oil contained its principal constituent of Eugenol.

The clove oil were obtained from Lancaster Chemical Company, UK and used as such for the spectral measurements. The room temperature Fourier transform IR spectra of title compounds were measured in the 4000 - 50 cm^{-1} region at a resolution of $\pm 1\text{cm}^{-1}$ using BRUKER IFS 66V Fourier transform spectrometer equipped with an MCT detector a KBr beam splitter and globar source. The Far IR spectrum was recorded on the same instrument using polyethylene pellet technique.

The Optimised energy structure is given in the Fig. 1.

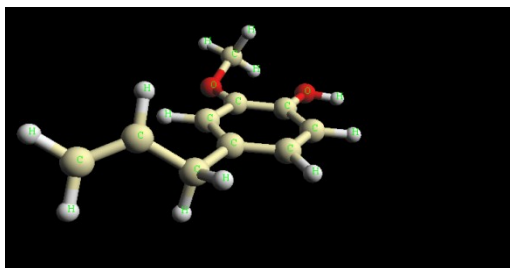


Fig.1.Optimisation of clove oil.

The Fig.2 shows the structure of *Aspergillus* fungai in bread. The experiment is done on the fungi by applying clove oil has its major constituents such as Eugenol. The FTIR study is also carried out to show the effect of clove oil before and after applying clove oil.

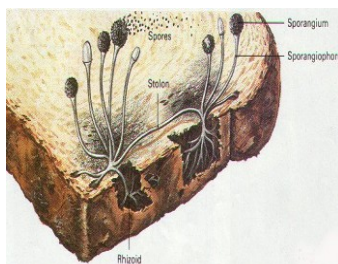
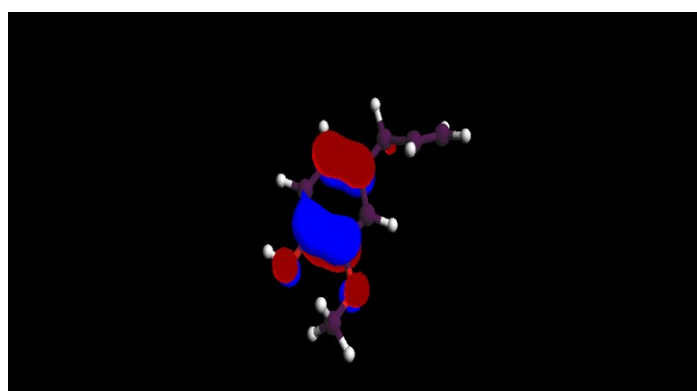


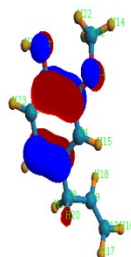
Fig.2.growth of Aspergillus fungai in bread

The florescent property of the clove oil also was carried to show the electron transition during the reaction clove oil on Aspergillus fungi.The Homo energy,Lumo energy of the molecule was also carried out to show the property of electron transfer.

Electron transformation in HOMO state



Electron spin polarization of clove oil



Vibrational analysis OF CLOVE OIL using FTIR METHOD:

Vibrational assignments in clove oil		Vibrational analysis of <i>Aspergillus</i> fungi in the presence of clove oil	
Frequency in cm	Assignment of the peak	Frequency in cm	Assignment of the peak
3942.46	O-H stretching	3343.20	O-H stretching
3822.69	O-H stretching	3179.59	O-H stretching
3717.77	O-H stretching	2923.45	O-H stretching
3604.20	O-H stretching	2163.71	C=C stretching
3498.57	O-H stretching	1637.31	C-H Finger print region
3390.71	O-H stretching	1515.58	C-C Stretching
2859.02	C-H Stretching	1439.41	C=H Bending

II. Results

- The above analysis discuss that the spectrum of clove oil. The wave frequency 3942.46 cm^{-1} is obtained at the transmittance range of 78.83%.
- Similarly the spectrum of *Aspergillus* fungi in the presence of clove oil, the wave frequency 3920.12 cm^{-1} is obtained at transmittance range of 36.23%.
- FTIR,UV Studies of clove oil shows the vibrational assignments of Eugenol ,and its fluoesent property .The application of clove oil with the property of aroma is also experimentally proved by the method of vibrational analysis
- The analysis spectrum of *Aspergillus* fungi in the presence of clove oil in bread is observed.The result shows that growthof *aspergillus* fungai is reduced because of the application of clove oil.

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