

SPECTROSCOPIC STUDIES (GEOMETRY OPTIMIZATION, E → Z ISOMERIZATION, UV/VIS, EXCITED STATES, FT-IR, HOMO-LUMO, FMO, MEP, NBO) OF NEW AZOMETHINE DYES FOR BIOLOGICAL APPLICATIONS

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Three new azomethine compounds have been predicted and synthesized. Their equilibrium geometric parameters, IR, NMR, UV/Vis and electronic absorption spectra have been presented and discussed.

Keywords: antioxidant activity, azomethine, electronic spectrum, geometry optimization.

In the present work the geometries and adsorption properties of the three new molecules were investigated by Density Functional Theory (DFT) in the solvent for the first time.

In the present work, first time the molecular structures of three newly synthesized azomethine dyes:

(1Z)-N-benzylidene-4-((E)-1-(oxim)ethyl)benzenamine,

4-((1Z)-4-((E)-1-(oxim)ethyl)phenylimino)methylphenol,

(Z)-1-(4-((Z)-4-methoxybenzylidene)amino)phenyl)ethanoneoxime have been investigated using Density Functional Theory (DFT/B3LYP/6-31+G*) in dimethylformamide (DMF). The electronic spectra of azomethine dyes in a DMF solvent was carried out by TD-DFT method. After quantum-chemical calculations three new azomethine dyes for optoelectronic applications were synthesized. FT-IR spectra of the title compounds are recorded and discussed. The computed absorption spectral data of the azomethine dyes are in good agreement with the experimental data, thus allowing an assignment of the UV spectra. The molecular HOMO-LUMO, excitation energies and oscillator strengths for E and Z isomers of the dyes have also been calculated and presented. Optical Properties of the PVA-films containing new substances have been also investigated[1].

BIBLIOGRAPHY

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A METHOD FOR IMRT TREATMENTS OF PROSTATE CANCER IMPROVEMENT

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The aim of the research work is to analyze modern methods in planning and elaboration of a new method for obtaining a volume-modulated dose distribution for irradiating prostate cancer by IMRT method.

Keywords: Radiation therapy, prostate cancer, IMRT, VMAT, medical linear accelerator, planning.