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UV-Visible absorption spectroscopy and Z-scan analysis along with corresponding molecular electronic structure analysis at DFT level for L-Tyrosine.

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Abstract:*Aqueous solutions of L-tyrosine prepared with a wide range of concentrations from 3.0 μM to 1.5 mMwere examined by UV-Visible spectroscopy and Z-scan analysis along with quantum mechanical calculation for its molecular structure for possible cause of linear and nonlinear optical activities. L-tyrosine has been found to absorb light at three regions around 193 nm, 224 nm and 275 nm in aqueous solution. These absorptions exhibit ^1L_a and^1L_btransitions in the side chain containing phenol ring structure. The aqueous solution of L-tyrosine also exhibits third order optical nonlinearity with negative refractive index of 3.18×10^{-8} m^2/W in the thermal regime as found by Z-scan technique. The HOMO-LUMO structure of L-tyrosine in solvated form calculated at DFT level using CAM-B3LYP parameters and aug-ccPVTZ /ccPVQZ basis sets give results consistent with observation of UV-Vis spectroscopy.*

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I. Introduction

UV-visible spectroscopy is one of the oldest modern technique used for electronic structure determination of compounds either in condensed phase or gaseous phase. This technique is based upon absorption of electromagnetic photons by atoms or molecules. As molecular orbitals are formed by overlapping of the adjacent atomic orbitals and further complicated by vibrational and rotational energy levels, the absorption spectra of molecules are not narrow as is in the case of elemental atomic spectrum, but rather consists of broad absorption bands whose peak positions and shapes are determined by structural features of absorbing material in question and its surrounding environment. Among the biomolecules, proteins and nucleic acids absorb light in the near UV and visible region of 150 - 800 nm. Except these others mostly absorb in the deep UV which are not experimentally suitable.

It has been found that the UV absorption in proteins comes mainly from the absorptions by the constituent aromatic amino acids L-tyrosine, L-tryptophan, L-phenylalanine [1-9] and also from cysteine disulfide bond[10,11]. Simple peptide structure containing only one type of the aromatic amino acid exhibits absorption pattern much like that of the constituent aromatic amino acid. Tryptophan absorbs most strongly having absorption peak at 280 nm with extinction coefficient of 5600 $L\ mol^{-1}cm^{-1}$and tyrosine at 275 nm with extinction coefficient 1400 $L\ mol^{-1}cm^{-1}$[12]. However, in case of human serum albumin (HSA) the contribution of L-tyrosine is expected to be more weighty compared to tryptophan as it is much more abundant (18:1) in the HSA structure[13]. Again its side chain chromophore phenol is more polar than the other aromatic chromophores and hence its absorbance is strongly influenced by the polar surrounding as it is exposed to the solvent[14]. Investigations on absorption by aromatic amino acids have been reported as early as 1883 which wereincomplete[1-5]. Katherinetal. in 1935 made extensive study on tyrosine, tryptophan and phenylalaninewhich produced somewhat different results than before[15]. Earlier absorption studies were made above 220 nm which was later extended up to 177 nm[3,16,17].

The absorption band position and intensity for the conjugated π-bonded systems depend strongly on the micro environment of the chromophores and the conformations of the respective molecules. It has been found that the absorption bands of tyrosine and tryptophan are redshifted by *1-3 nm*when incorporated in protein structure[6,7,9]. In particular cases, the absorption patterns have been directly correlated to its structural features. As a part of optical study of HSA we need to look at the different linear and nonlinear optical responses of tyrosine as well as the others.During absorption of electromagnetic photon a range of incidents take place in sequence like electronic excitation followed by charge redistribution, reorganization of dipole moment,