

SPECTROSCOPIC INVESTIGATION AND PREDICTION OF LASER ACTION PROPERTIES OF 4-HYDROXYCOUMARIN DYE IN SOLGEL

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Out of thousands of organic dyes synthesized over the last hundred years only a few show laser action when excited by Q-switched laser or a pulsed nitrogen laser and still fewer under flash lamp excitation. Organic dyes that show laser action are selected by trial and error. For an efficient working of a laser material it is important to select dyes which have high quantum yield and low lasing threshold. Coumarins or 6-benzopyrones are known for their strong lasing effect. It is a class of laser dyes emitting in the blue green region of the spectrum and derived from coumarin - the parent molecule on substitution with auxochromic (OH, NH₂, CH₃, etc.) groups at various carbon positions. Depending on the location and direction of the singlet-singlet (S-S) relative to triplet-triplet (T-T) oscillators within the molecular frame, substitution by the hydroxy auxochromic group may cause T-T absorption bands to move in or out of fluorescence region, or they may be left unchanged. An attempt is made to study the spectroscopic characteristics of 4-hydroxycoumarin molecule. Electronic absorption spectra of 4-hydroxycoumarin are measured in the wavelength region 200-700 nm in liquid solvents and solgel. Fluorescence spectrum is measured on exciting 4-hydroxycoumarin doped in solgel by varying the excitation wavelengths. Electronic transitions observed experimentally, are interpreted using the optimized geometries and CNDO/S-CI method. Assignments of observed electronic transitions are made on the basis of singlet-triplet electronic transitions. Further, effect of hydroxy substituent on the spectral properties of the parent aromatic molecule are investigated on the basis of molecular structure and spectral predictions for 4-hydroxycoumarin as a potential dye laser material are made. These predictions supported by theoretical results are presented graphically with possible arrangements of low energy S-S oscillators relative to T-T oscillators located in the fluorescence region. Depending on short or long axis substitution, the redshifts of the S-S and T-T absorption bands are observed and the importance of these red shifts, as related to the laser action properties are discussed. We found a good agreement between the experimental and calculated results. Further more, 4-hydroxy coumarin doped in solgel is found to be a potential dye laser material.