Principal Component Analysis for Imidazo[4,5-b]pyridine Linear and Non-Linear Optical Properties Description

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Two-photon absorption (TPA) is a non-linear optical phenomenon that is extensively studied and employed in different fields of photonics. Several materials with good absorptive and emissive properties can be used as a nonlinear medium. These materials include organic molecules such as fluorophores and chromophores with extended π-conjugated systems, nanomaterials like quantum dots, nanorods, and graphene, as well as inorganic materials like doped semiconductors [1]. The efficiency of the TPA process in a material depends on numerous factors, including the type of material, electronic structure, solvent used, thermic and chemical properties, and others [2]. In addition, when analyzing optical systems using non-linear spectroscopy, a significant amount of data and variables that are not easily interpretable or correlated are involved. Multivariate analysis techniques simplify the treatment and interpretation of large data sets. Principal Component Analysis (PCA) is a commonly used method for reducing and exploring large databases [3]. PCA reduces an original space of p variables and n observables into a subspace of X_n linear combinations named principal components. This work used PCA as a multivariate analysis technique to simplify and interpret the one- and two-photon absorption spectra and the photophysical properties data obtained in the nonlinear characterization of six Imidazo[4,5-b]Pyridine [4]. The results show that PCA can reproduce the experimental results with a cumulative variance of up to 95%. Additionally, linear regression was used to investigate the dependence of the Two-Photon Absorption cross-section (TPACS) intensity on different photophysical parameters. The regression model indicates that the first and second excited state transition dipole moments, permanent dipole moment, and fluorescence quantum yield dominate the behavior of TPACS, showing high correspondence with the experimental behavior observed.

References

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