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3.Massoud Kaykhaii







SPECTROSCOPIC STUDY OF THE MOLECULAR ASSOCIATION OF BERBERINE AND PALMATINE

G. K. Kasimova
Ch.A.Nematjonova
Asia International University, Uzbekistan
E-mail: guzal.kasimova.85@mail.ru
M. A. Makhmudova
Bukhara State Technical University, Uzbekistan
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Berberine and palmatine are natural isoquinoline alkaloids characterized by an extended conjugated system and pronounced spectral properties in the ultraviolet and visible regions. The electronic structural features of these compounds determine their ability to participate in various types of intermolecular interactions. In solutions, such interactions may lead to molecular self-association and the formation of aggregated structures, which is reflected in the electronic and polarization-spectral characteristics of the systems under investigation [1–3].

The study of molecular association processes is of particular interest for biologically active compounds, since the formation of molecular associates can alter their optical, photophysical, and physicochemical properties. The structural similarity between berberine and palmatine enables a comparative investigation of the patterns of their intermolecular interactions and an assessment of the influence of molecular structural features on aggregation processes [4–6].

The aim of the present study was to investigate the spectral manifestations of intermolecular interactions between berberine and palmatine and to elucidate the specific features of their molecular association using electronic and polarization spectroscopy techniques. To achieve this objective, the spectral characteristics of berberine and palmatine solutions were investigated under varying conditions affecting intermolecular interactions. Particular attention was paid to the positions and intensities of electronic absorption bands, changes in spectral band profiles, and the polarization characteristics of the investigated systems.

Polarization measurements were performed using a Spektropol-1 spectropolarimeter over the wavelength range of 200–610 nm. Additional information on the optical anisotropy of the molecular systems was obtained using a Jasco-20 dichrograph operating in the spectral range of 200–700 nm. To detect weak manifestations of optical anisotropy, an optical system incorporating a double Fresnel parallelepiped was employed, enabling the transformation of light polarization states [7].

The Jasco-20 electro-optical system employs a Pockels cell containing a KDP (KH_2PO_4) crystal. This experimental configuration enables the detection of small differences in the absorption of polarized light components, thereby revealing changes associated with the spatial organization of molecules within the resulting molecular associates. The high sensitivity of the methods employed is particularly important for investigating weak intermolecular interactions.

Analysis of the electronic absorption spectra of berberine and palmatine makes it possible to monitor changes in spectral parameters accompanying an increase in the

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extent of intermolecular interactions. Variations in solution concentration may lead to deviations from the spectral characteristics typically observed when molecules exist predominantly in their monomeric state. Such changes may be manifested as a redistribution of absorption band intensities, alterations in band shapes, and shifts in their spectral positions.

The observed spectral changes may be associated with a decrease in the average intermolecular distance and an enhancement of interactions between the conjugated chromophoric systems. The planar regions of the molecular structures of berberine and palmatine provide favorable conditions for interactions between their π-electron systems. Therefore, one possible mechanism of aggregate formation involves π–π stacking interactions between neighboring molecules. In addition, electrostatic interactions and solvent properties may influence the stability of the resulting structures [8,9].

A comparative investigation of berberine and palmatine is of particular interest because of their closely related molecular structures, despite certain differences in their substituents. These structural features may affect electron density distribution, the spatial proximity of molecules, and the stability of the resulting molecular associates [10]. Consequently, even relatively minor changes in chemical structure may lead to differences in the electronic and polarization spectra of the two compounds. In this context, polarization-spectroscopic methods complement conventional electronic spectroscopy. While electronic absorption spectra primarily provide information about changes in the electronic energy states of chromophoric systems, polarization measurements offer additional insights into the orientation of interacting molecules and the optical anisotropy of the resulting supramolecular structures.

The observed relationships indicate the potential of combining electronic and polarization spectroscopy for investigating the molecular association of natural alkaloids. Comparison of the spectral characteristics of berberine and palmatine makes it possible to assess the influence of molecular structure and environmental conditions on the nature of intermolecular interactions. Thus, the spectroscopic approach enables the identification of changes in the molecular states of berberine and palmatine associated with enhanced intermolecular interactions and the formation of associated structures. Combined analysis of electronic and polarization characteristics provides broader opportunities for elucidating the mechanisms of self-association of these biologically active compounds.

The results of such investigations may be of interest for studying photostability, developing pharmaceutical formulations, and establishing relationships between molecular organization and the physicochemical properties of natural alkaloids.

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