

Unraveling environmental effects in the absorption and fluorescence spectra of *p*-methoxyphenylpiperazine derivatives

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Streszczenie

The *p*-methoxyphenylpiperazine motif can be found in many biologically active molecules, including approved drugs. It is characterized by a relatively weak fluorescence, which can be employed in different types of studies involving molecules with this motif. In this work, a thorough analysis of the absorption, excitation and emission spectra of the diphenyl(aminomethyl)phosphine and tris(aminomethyl)phosphine derivatives of *p*-methoxyphenylpiperazine, supported by the DFT calculations (ω B97XD/6-311++G(d,p)) with NBO and QTAIM analysis also for different model molecules (e.g. 1-(4-methoxyphenyl)-4-methylpiperazine) enabled determination of the mechanisms underlying beneath the electronic transitions and allowed to rationalize mixed solvent effects observed in electronic spectra of the studied compounds. Electronic transition from the ground state to the first excited state can be regarded as the $n, \pi \rightarrow \pi^*$ transition with no solvatochromic effects, however the hydrogen bonds between the HBD solvent molecules and the nitrogen atom bound directly to the aromatic ring (N(4)) are shifting strongly the 1st absorption or excitation band maxima to the higher energies. Fluorescence band, as a result of the electron transition from the equilibrated 1st excited state to the ground state, can be described as the $\pi^* \rightarrow \pi$ with positive solvatochromism. N(4) in the excited states adopts a sp^2 hybridization and is no longer able to form HBs. On the other hand, increased electron density on the aromatic ring makes the emission processes vulnerable to its direct environment.

Słowa kluczowe

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