Effect of solvent polarity on photophysical parameters of 3-aminoflavone.

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Photophysical behavior of 3-amino flavone (3AF) in different media has been studied using steady state and time-resolved fluorescence spectroscopy in combination with DFT and TD DFT B3LYP/6-31G (d,p) calculations involving the ground and the excited state geometry optimization. Comparison of experimental solvatochromic shifts with the calculated energies in different solvents (PCM model) allows to conclude that the excited state of 3AF, corresponding to the $\pi \rightarrow \pi^*$ ($S_0 \rightarrow S_1$) transition, has a partial CT nature. The lifetime and quantum efficiency measurements in function of solvent polarity shown that in weakly polar solvents the radiationless rate constant is very high. On the basis of TD DFT calculations for singlet and triplet state distribution in different environments (PCM model) we hypothesize that in weakly polar solvents the intersystem crossing may be a prevailing relaxation process.

Słowa kluczowe

3-Amino flavone, Fluorescence, DFT and TD DFT calculations, PCM model, electron transfer, Lifetimes, CT states, Triplet states

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