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Spectral and photophysical properties of cytisine in acetonitrile – theory and experiment

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Abstract: Spectral and photophysical properties of (–)-cytisine that is used as a smoking cessation aid, and which derivatives are promising tools in a treatment of neurological diseases, were investigated in acetonitrile, non-specifically interacting solvent with a polarity similar to water. The two chair conformers of cytisine were found the most stable in the ground state S_0 and the lowest excited singlet state $S_1(\pi,\pi^*)$, wherein axial one was characterized by a significantly larger abundance, fluorescence lifetime 0.15 ns and fluorescence quantum yield 0.008. The $S_1(\pi,\pi^*)$ excited state of both cytisine conformers deactivated almost exclusively via internal conversion.

Keywords: cytisine, UV-VIS, fluorescence, conformers