STRUCTURE AND LUMINESCENT PROPERTIES OF THE DERIVATIVES OF 4-ARYLIDENE-2-ARYL-OXAZOLONE-5 IN SOLUTIONS AND IN THE CRYSTALLINE STATE

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Following derivatives of azlactones (4-arylidene-2-aryl-oxazolone-5) were studied for their luminescent properties in solutions and crystalline states.

\begin{align*}
\text{Ar} & \quad \text{Ar}' \\
I & \quad \text{Phenyl} \quad \text{Phenyl} \\
II & \quad p\text{-Anisyl} \quad \text{Phenyl} \\
III & \quad p\text{-N,N-Dimethylaminophenyl} \quad \text{Phenyl} \\
IV & \quad o\text{-Hydroxyphenyl} \quad \text{Phenyl} \\
V & \quad 2\text{-Hydroxy-1-naphthyl} \quad \text{Phenyl} \\
VI & \quad 2\text{-Hydroxy-1-naphthyl} \quad o\text{-Tolyl}
\end{align*}

Fluorescence quantum yields of azlactones were in the range of 0.0001-0.0234 in solutions, but these values are found to increase 10-1000 times of magnitude in crystalline state. This observation is related to the flattening of oxazolone-5 molecules while packing into the crystal lattice, that makes impossible any intramolecular rotations and movement. Azlactones IV to VI have exhibited low efficient excited state proton transfer reaction rate constant of 1x10\textsuperscript{-11}s\textsuperscript{-1} in crystalline state. The quantum-chemical calculations show the possible reasons of photochemical instability of the derivatives belong to oxazolone-5 series: the photochemical Z-E isomerization around the double C=C bond on position 4 of the heterocycle and the azlactone cycle cleavage in the \textit{\textalpha} -position to the carbonyl group. In acidified solutions very rapid photochemical reaction, is found to lead to the damage of conjugated system of oxazolone molecule and results in considerable short-wavelength shift in the absorption spectra.