

BODIPY KETONES AS PROMISING PHOTOINITIATORS AND DYES FOR PHOTOAFFINITY LABELING

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Benzophenone is a well-known photoinitiator of radical processes. Under UV irradiation it forms diradicals [1]. This property is used for photopolymerization, surface formation and labeling [2-4]. Today fluorescence is found effective and implements new methodologies. At the same time, BODIPY's are some of the most popular fluorophores and are used for diverse applications. To the best of our knowledge, only one research where BODIPY-phenylketones (BPK) photoactivity mentioned is published [5]. DFT and TDDFT calculations were held in ORCA 4.2.0 with PBE functional, ma-def2-SVP basis set without solvation. Density fitting, dispersion correction, and enhanced integration grid were applied. In a first approximation, an assumption could be made that the propensity to the T₁ formation directly correlates with the conditions of S₀→S₁ transition due to the intersystem crossing. The efficiency of photoactivation depends on the absorption intensity, so only the first dominant transition will be discussed. For benzophenone such is at 316 nm. It corresponds to the HOMO-1→LUMO excitation. Transitions for considered 1-, 2- and 3-benzoyl-8-methylBODIPY have complex nature and mainly contributed by HOMO-1→LUMO and HOMO→LUMO excitations. For presented BPK's the excitation energy is in the range of 415-437 nm. Thus, BPK can be photoactivated by less energetic light than benzophenone does. In our further works, the synthesis and characterization of described compounds are planned as well as the design and more thorough computational study of other BPK's.

References:

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