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Substituent Effect on the Formation of the Inclusion Complex as Guest Molecules of 2-Pyridones and Its Photochemical Reactivity in the Solid State.

MASAYUKI KUZUYA*, AKIHIRO NOGUCHI, NAOHISA YOKOTA,
TAKACHIYO OKUDA, FUMIO TODA, KOICHI TANAKA

Various substituted 2-pyridones [1] and the 1-methylated compounds [2] were included as guest molecules in a host molecule, 1,1,6,6-tetraphenyl-2,4-hexadiyne-1,6-diol (TPH). The tautomeric 2-pyridones [1] bearing polar substituents at C-6, which favor the 2-pyridinol form in solution, existed exclusively as the 2-pyridone form in the inclusion complexes. The photodimerizations of [1] and [2] in solid state of the inclusion complex were also investigated. Only unsubstituted [1a] gave efficiently the trans-anti dimer among [1], while most of [2] gave efficiently and stereo-selectively the corresponding dimers.

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Nature of Substituent Effect of Nitro and Methoxyl Group on Photocycloaddition of Polymethylene Dicinnamates.

MASAYUKI KUZUYA*, NAOHISA YOKOTA, AKIHIRO NOGUCHI, TAKACHIYO OKUDA

The nature of the nitro substituent effect and topotactic assistance by the polymethylene chain of polymethylene dicinnamates upon the rate of photocyclization and the stereochemistry of photoproducts have been explored, a striking rate enhancement and stereospecificity of the photoproduct were observed on a trimethylene dicinnamate derivative. Based on the results of the CNDO/S-CI excited state calculation of the model compounds, it is concluded that the acceleration character of the nitro substituent is mainly due to the odd electron density at the reaction site, i. e. the olefinic double bond; it is not due to the facile exciplex formation on the excited singlet state, unlike that of a methoxyl substituent.

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Mechanistic Insight into Immobilization and Release of Active Radical Species on a Novel Plasma-Driven Ultrathin Film.

MASAYUKI KUZUYA*, MASAHARU NAKANISHI, SACHIIHIKO NAKAI

Mechanism for immobilizing an active radical species and permitting its slow release on a novel plasma-driven ultrathin film was proposed with the aid of molecular orbital calculations of some model compounds as well as taking a characteristics of a plasma process for the film deposition into accounts, which involves the existence of non-optimized carbon-centered bonds in rehybridization in the embryonic ultrathin film so that the film is forced to contain some nonoptimal units, i. e. weakened σ -bonds with strain and/or torsion and the propensity of their facile bond-cleavages.