Solvent effect on the quenching of singlet oxygen by 3-methylindole

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Detection of O2(1?g) emission, ?max = 1270 nm, following laser excitation and steady-state methods were employed to measure total, kT, and chemical, kR, reaction rate constants for the reaction between 3-methylindole and singlet oxygen in several solvents. Values of kT range from 0.12 ± 0.008 × 107 M-1s-1 in n-heptane to 32.0 ± 1.12 × 107 M-1s-1 in D2O at pD = 7.4. Analysis of the solvent effect on kT by using the semiempirical and theoretical linear solvent free-energy relationship (LSER and TLSER) solvatochromic equations indicates that singlet oxygen deactivation by 3-methylindole is accelerated by solvents with large ?* values. This result supports the participation of an exciplex intermediate with partial charge transfer character, leading to either chemical reaction or physical quenching. The contribution of chemical reaction to total quenching depends significantly on the solvent. Chemical reaction can be neglected in non-polar solvents, whereas in hydrogen-bond donor solvents,