Supplementary Information

TPPS$_4$—Sensitized Photooxidation of Micropollutants—Singlet Molecular Oxygen Kinetic Study

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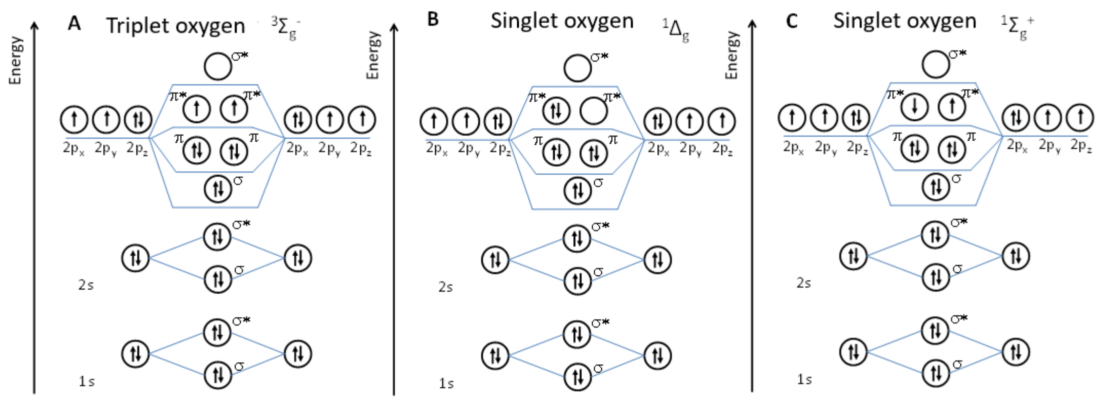

Figure S1. Distribution of electrons in the molecular orbitals of oxygen in the ground and singlet states. Arrows symbolize electrons, electron spins are marked with arrows.

Table S1. Lifetime of $^1\Delta gO_2$ in different solvents [8,15,21,29].

solvent	τ_Δ, µs	$k_d\times10^{-4}$, 1/s	solvent	τ_Δ, µs	$k_d\times10^{-4}$, 1/s
H_2O	3.3	50±20	**C_2H_3N**	75	3.3±0.7
D_2O	67	3.0±0.2	**CH_2Cl_2**	94	1.6±0.7
$C_6H_5CH_3$	30	4.0	**$CHCl_3$**	247	0.44±0.18
CH_3OH	10.4	14±2	**CS_2**	34 000	0.5±0.15
C_6H_6	31	4.2±0.9	**C_6D_6**	700	0.27±0.06
$C_2Cl_3F_3$	99 000	-	**C_6F_6**	3900	0.17±0.6

Table S2. Constant rates of singlet oxygen reactions with physical and chemical quenchers.

Quencher	Quenching type	Rate constant $M^{-1}\ s^{-1}$	Reference
NaN_3	physical	$k_q = 4.78\times10^8$ (D_2O)	[30]
		$k_q = 2\times10^9$ (H_2O)	[31]
		$k_q = 2.8\times10^9$ (CH_3CN)	[30]
DABCO		$k_q = 1.2\times10^7$ (H_2O)	[31]
imidazole		$k_q = 2\times10^7$ (D_2O)	[32]
β-carotene		$k_q = 1.4\times10^{10}$	[28]
likopen		$k_q = 3.1\times10^{10}$	
Histidine	Physical and chemical	$k_q = 5\times10^7$	[28]
1-methyl-cyclopentane	chemical	$k_r = 2.1\times10^5$ (CH_3OH)	[29]
4-methyl-cyclohexane		$k_r = 3.1\times10^3$ (CH_3OH)	

3-methylstyrene	$k_r = 5.0×10^6$	
2-phenylfuran	$k_r = 9×10^6$ (H_2O)	[11]
2-chlorophenol anion	$k_r = 1.9×10^8$ (H_2O)	