

CHEMPHYSICHEM

Supporting Information

Unraveling the Degradation Mechanism of Purine Nucleotides Photosensitized by Pterins: The Role of Charge-Transfer Steps

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**On the mechanism of the degradation of purine nucleotides
photosensitized by pterins: a radical charge-transfer model**

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Supporting Information

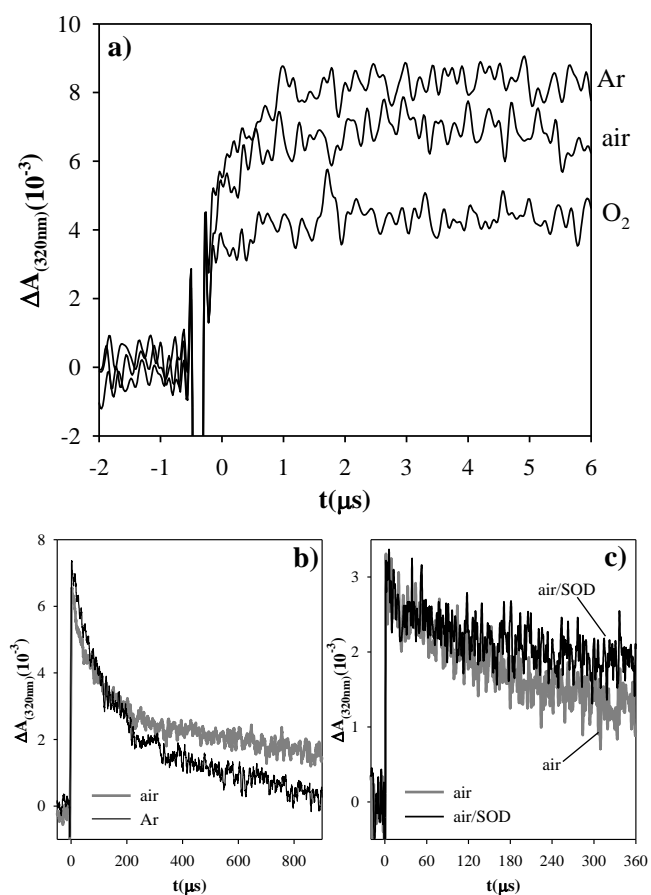


Figure S1. Formation (a) and the subsequent evolution of dGMP(-H)' (b and c) monitored by the time-evolution of the ΔA at 320 nm after the laser pulse at various O_2 concentrations. Experiments performed in Ar- and O_2 -saturated aqueous solutions and in air-equilibrated solutions in the absence and in the presence of SOD (50 U/mL). Excitation wavelength 355 nm, $[\text{Ptr}] = 100 \mu\text{M}$, $[\text{dGMP}] = 1 \text{ mM}$.

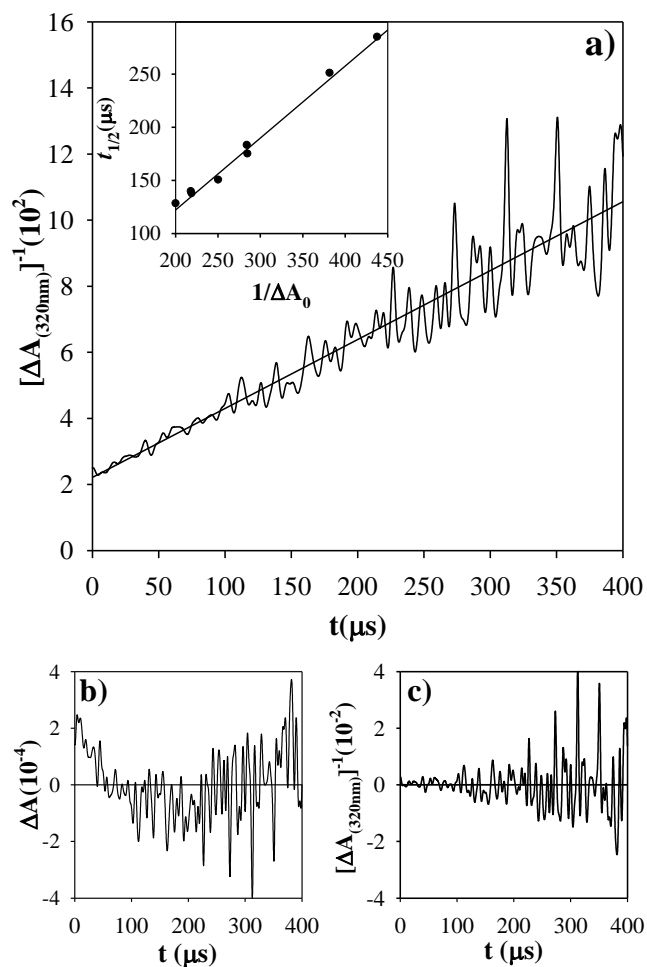


Figure S2. Decay of dGMP(-H)' monitored by the time-evolution of the ΔA at 320 nm after the laser pulse in Ar-saturated aqueous solutions. a) Plot of ΔA^{-1} vs. time. Inset: Dependence of $t_{1/2}$ with the initial amount of radical formed evaluated as ΔA^0 . Excitation wavelength 355 nm, $[Ptr] = 100 \mu\text{M}$, $[dGMP] = 200 \mu\text{M}$. Residuals analysis: b) first order fit, c) second order fit.

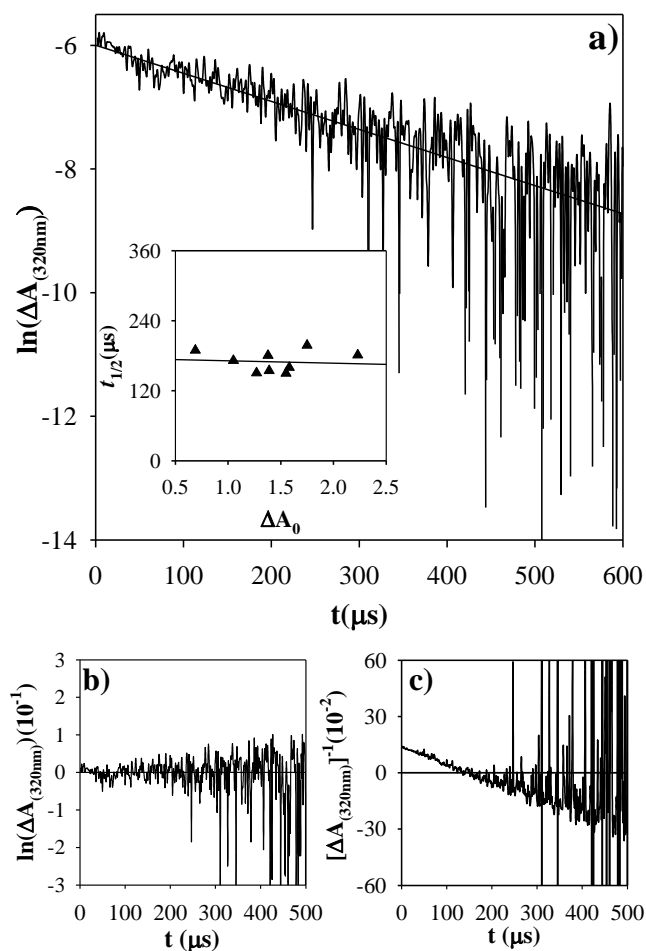


Figure S3. Decay of dGMP(-H)• monitored by the time-evolution of the ΔA at 320 nm after the laser pulse in air-equilibrated aqueous solutions in the presence of SOD (50 U/mL). a) Plot of $\ln(\Delta A)$ vs. time. Inset: Dependence of $t_{1/2}$ with the initial amount of radical formed evaluated as ΔA^0 . Excitation wavelength 355 nm, [Ptr] = 100 μM , [dGMP] = 100 μM . Residuals analysis: b) first order fit, c) second order fit.

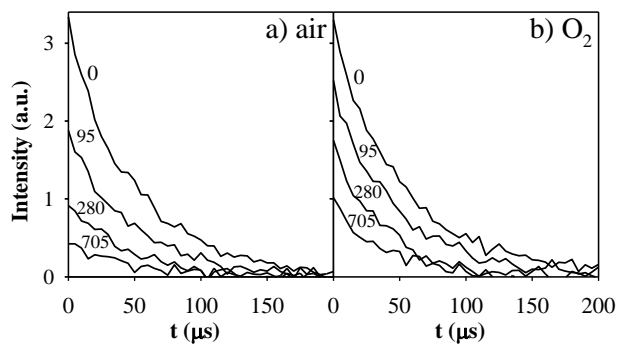


Figure S4. Time-resolved $^1\text{O}_2$ experiments: quenching of $^1\text{O}_2$ emission by dGMP. Experiments performed in D_2O solutions containing Ptr and dGMP at pD 5.5; excitation wavelength 340 nm, [Ptr]= 200 μM . a) and b) Selected NIR emission decays in the absence and in the presence of various concentrations of dGMP (above each decay (μM)) in air-equilibrated and O_2 -saturated solutions, respectively.

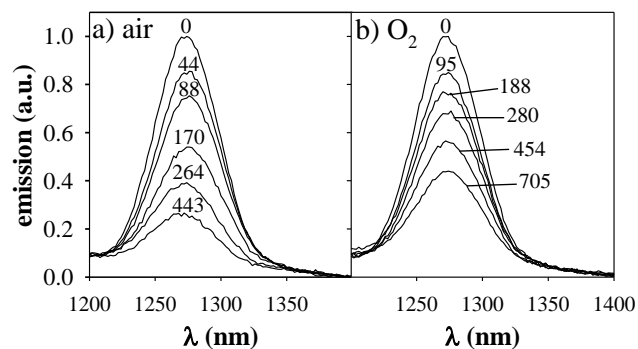


Figure S5. Steady-state $^1\text{O}_2$ experiments showing quenching of the emission of $^1\text{O}_2$ by dGMP performed in D_2O solutions containing Ptr and dGMP at pD 5.5. a) and b), selected NIR emission spectra registered in the absence and in the presence of various concentrations of dGMP (indicated above each spectrum (μM)) in air and O_2 -saturated solutions, respectively. Excitation wavelength 350 nm, $[\text{Ptr}] = 200 \mu\text{M}$.