Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Relaxation Pathways of the Biologically Relevant Pterin Chromophore

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Electronic Supplementary Information

1. Calculated Ground-State Tautomers Energies

Table S1. Predicted ground-state stabilization energies (eV) for the two lowest-energy tautomers of pterin at pH 10.5 (see Scheme 1) in water at the X/IEF-PCM/6-311++G(d,p) level of theory[a]

X	1a	1b
B3LPY	0.00	0.31
CAM-B3LYP	0.00	0.34
M052x	0.00	0.36
PBE1PBE	0.00	0.32
MP2	0.00	0.41

[a] where X stands for the functional.

2. Time-Resolved Absorption Spectroscopy

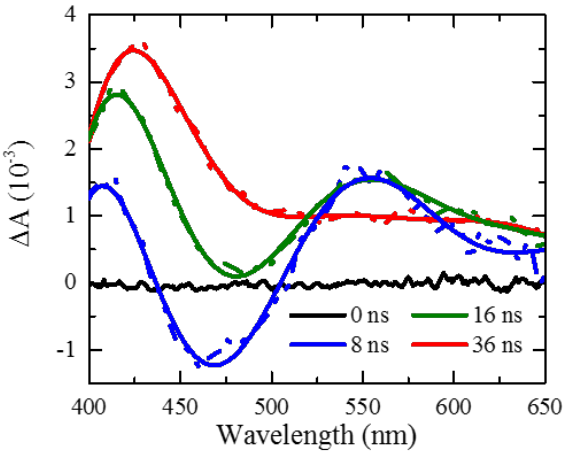

Figure S1. Nanosecond transient absorption spectra of **1a** in aqueous borate buffered solution at pH 10.5 under ambient (air) conditions. The experimental data is shown with the dashed lines. Solid curve lines are shown for clarity (i.e., as a guide to the eye).

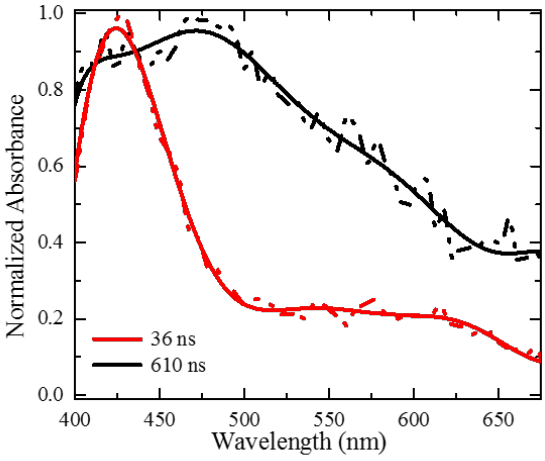

Figure S2. Normalized nanosecond transient absorption spectra of the two long-lived species of **1a** in aqueous borate buffered solution at pH 10.5 under ambient (air) conditions. Showing maximum triplet signal (red) and the maximum neutral radical signal (black). The experimental data is shown with the dashed lines. Solid curve lines are shown for clarity (i.e., as a guide to the eye).

3. Stern-Volmer Plot

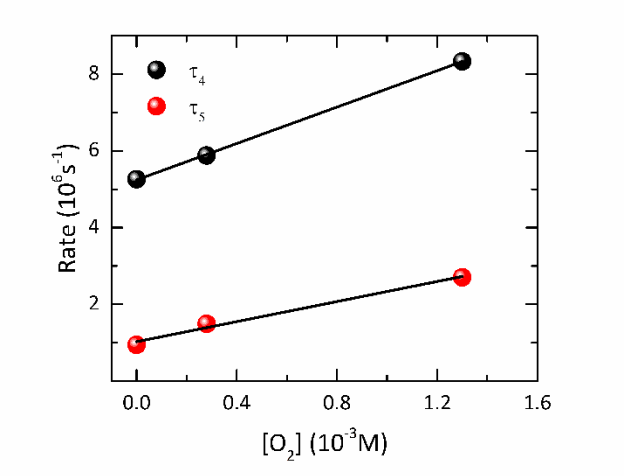

Figure S3. Stern-Volmer plots of the decay rate for the two long-lived transient species of **1a** in aqueous buffered solution at pH 10.5 (see Table 2) as a function of oxygen concentration in solution.