Supporting Information

Oxidation of Bromide Ions by Hydroxyl Radicals: Spectral Characterization of the Intermediate $BrOH^{\bullet-}$

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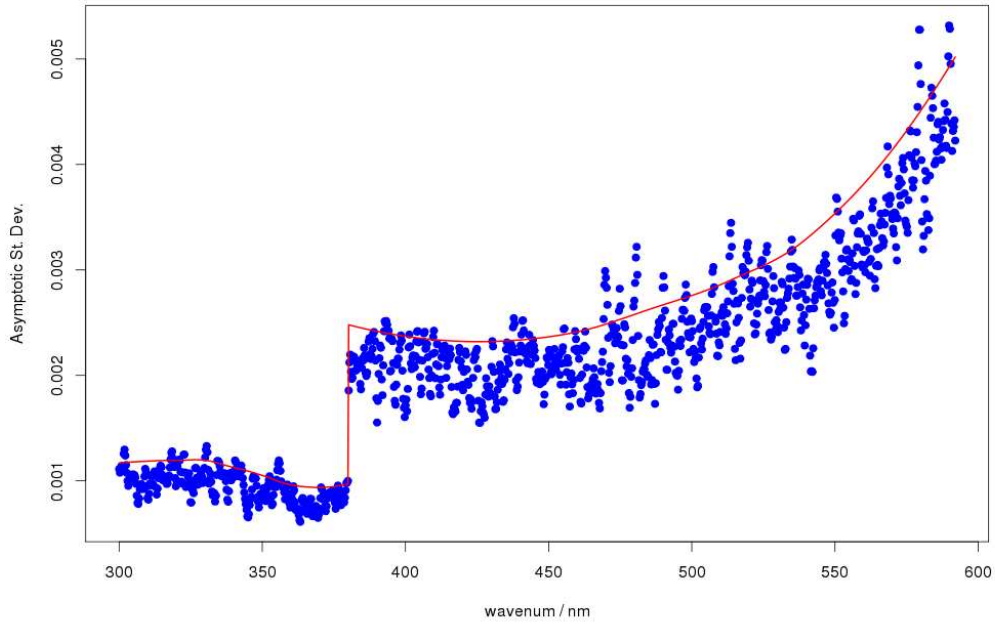

Figure S1: Wavelength-dependence of noise in data. The dots are the standard deviation calculated over 200 points at late time/delay. The red curve represents the 90% probability upper bound for the noise amplitude.

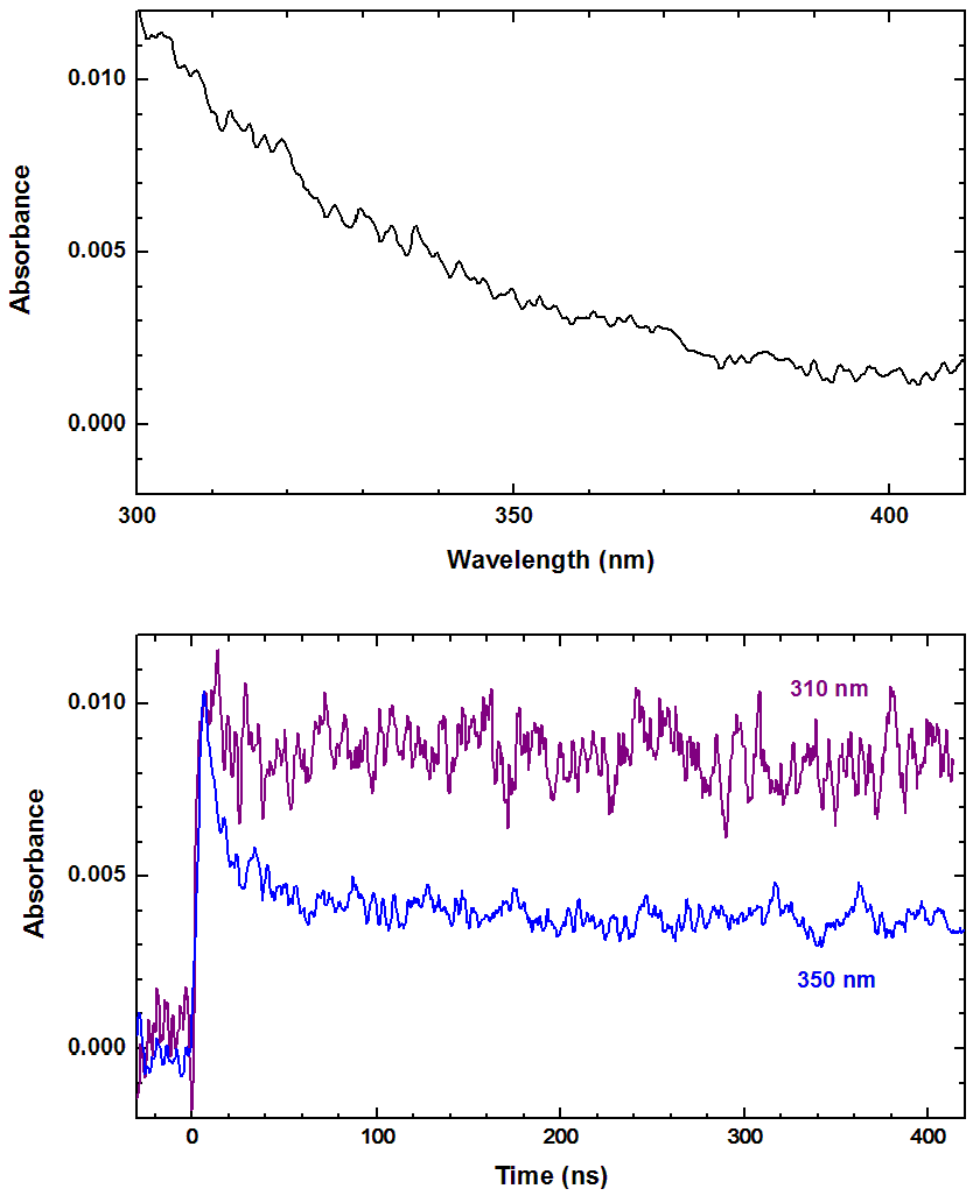

Figure S2: Optical absorption spectrum (top) and time-dependent signals (bottom) obtained by pulse radiolysis of Ar-purged aqueous solutions containing 0.1 M acetone.

The found spectrum corresponds to that of the protonated radical, $(CH_3)_2C^{\bullet}OH$, generated by the reaction between acetone and hydrated electron (R8-9), as reported in the literature (Kasama, K.; Takematsu, A.; Arai, S. *J. Phys. Chem.* **1982**, *86*, 2420-2427; Mills, G.; Henglein, A. *Radiat. Phys. Chem.* **1985**, *26*, 391-399). The fast rise in absorbance during the pulse duration is due to the solvated electron. Then, the disappearance of the solvated electron is observed at 350 nm where its extinction coefficient is greater than that of $(CH_3)_2C^{\bullet}OH$, but it is not detected at 310 nm where the extinction coefficients are similar.

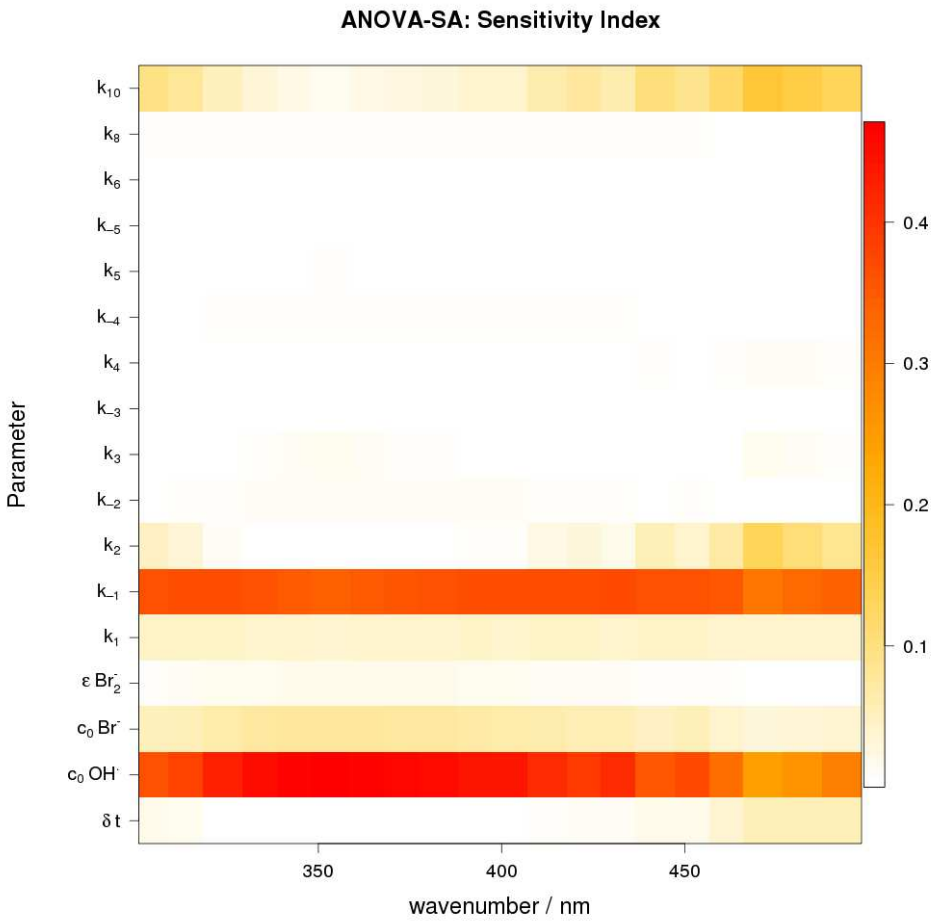

Figure S3: Sensitivity map.

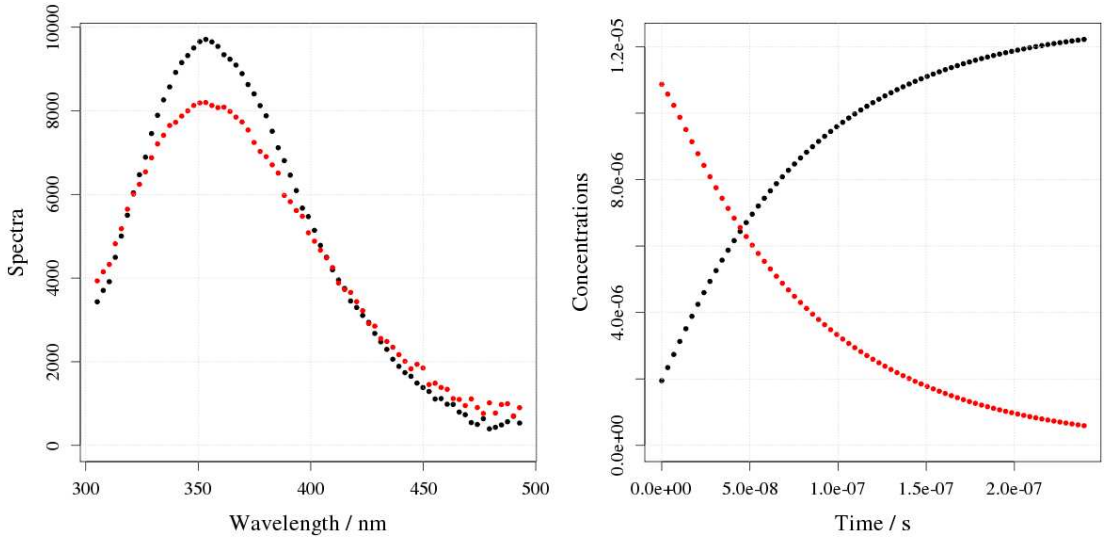

Figure S4: Absorption spectra (in dm^3 mol^{-1} cm^{-1}, left) and concentrations versus time (in mol dm^{-3}, right) of $Br_2^{\bullet-}$ (black dots) and $BrOH^{\bullet-}$ (red dots) obtained with the optimal set of parameters MAP2 during the Bayesian data analysis of the experimental results in Figure 1.

Full references

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