Illuminating the photoisomerization of a modified azobenzene single crystal by femtosecond absorption spectroscopy

Supplementary Material

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Crystal structure:

The crystal structure for (1,2-bis(8-bromo-6-methoxy-2,3-dihydrobenzo[b][1,4]dioxin-5-yl) diazene) can be found on the Cambridge Crystallographic Data Centre (DOI: 10.5517/ccdc.csd.cc1p70wt). The space group is P $2_{1/c}$, with crystals growing in the orthorhombic crystal habit. Crystals of roughly 5 x 5 x 5 cm were big enough to easily identify

the (011) face by eye. The crystals were positioned with the (011) face at the cutting plane.

Residuals of DAS fit:

The 2D residuals map is shown below. The residuals were calculated by taking the difference between the data reconstructed with the same number of SVD components used in the fit and the global analysis (GA) fit itself, as higher order components contain noise originating from the laser.

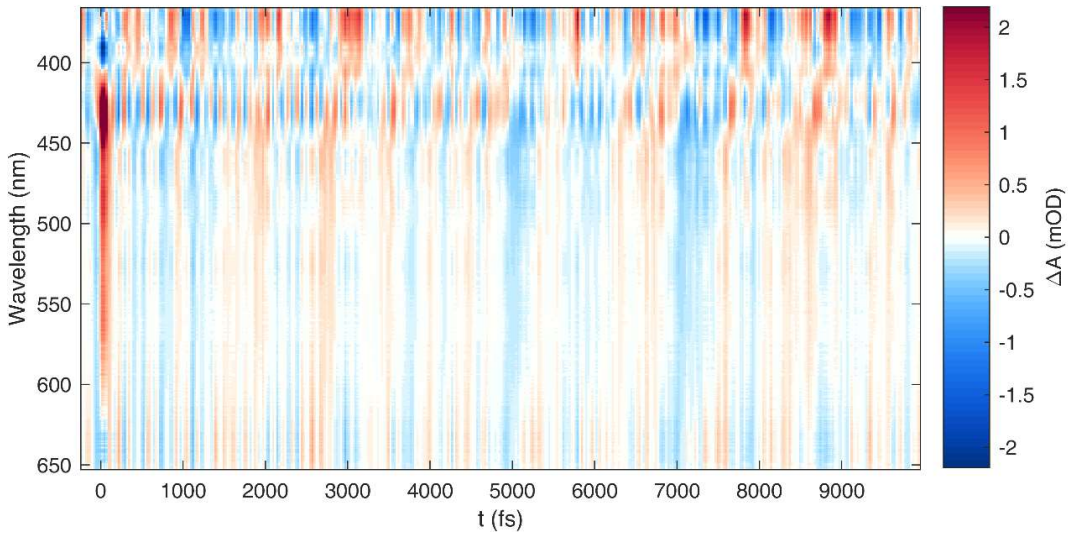

Fig. S1: The 2D residuals map taken as a difference between the raw data and the GA fit. The raw data was reconstructed using the same number of SVD components as used in the GA fit.

Select wavelengths of the 2D residuals map have been plotted below in Figs. S2 – S4. Traces have been shown starting at + 300 fs, due to the presence of a cross-phase modulation signal around t = 0 fs, to illustrate the presence of oscillatory signal. Traces at 390, 430, and 610 nm have been selected to showcase the oscillations in the residuals. We highlight that the individual traces appear to be noisy, but oscillatory dynamics are more resolvable in the Welch spectral power estimate as seen in Fig. 9 of the paper.

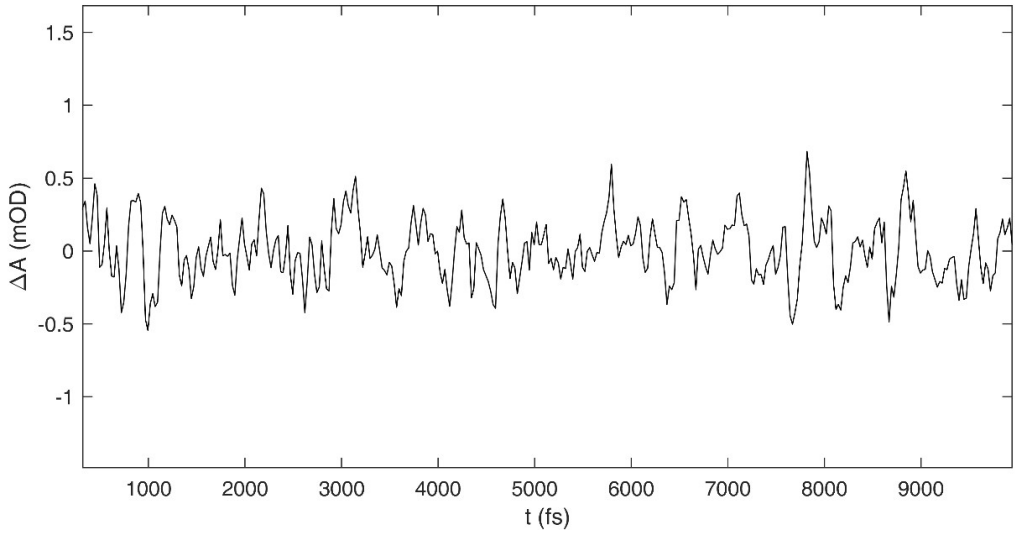

Fig. S3: The residual trace at 390 nm, shown from t = 300 fs and on.

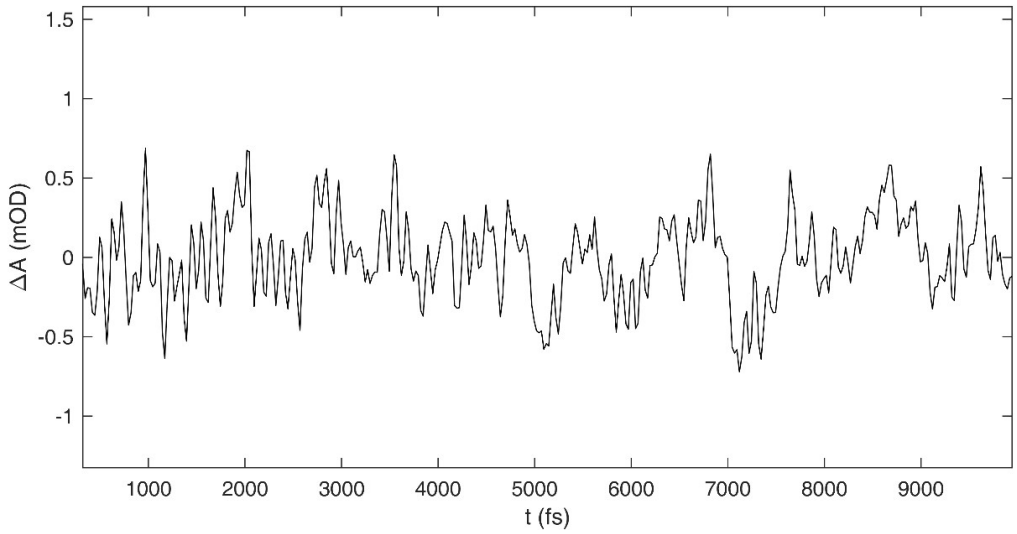

Fig. S4: The residual trace at 450 nm, shown from t = 300 fs and on.

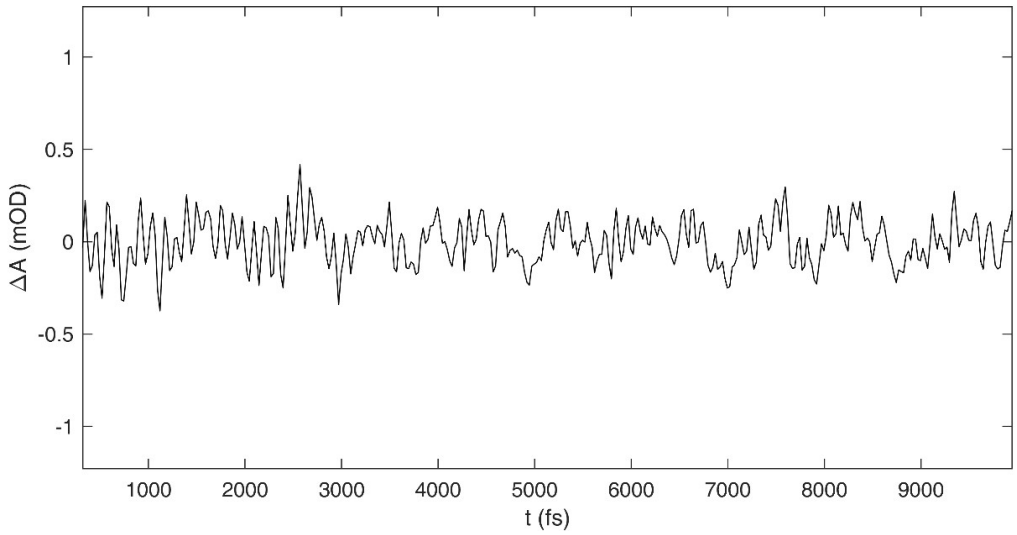

Fig. S5: The residual trace at 610 nm, shown from t = 300 fs and on.

The Welch spectral power estimate seen in Fig. 9 was performed on the 2D residuals map at t > 300 fs to prevent influence from the cross-phase modulation signal seen around t = 0 fs.