Supporting Information

An All-Photonic Molecule-Based D Flip-Flop

Patricia Remón,[†] Magnus Bälter,[‡] Shiming Li,[‡] Joakim Andréasson,[‡,] and Uwe Pischel[†,]**

[†] Centre for Research in Sustainable Chemistry and Department of Chemical Engineering, Physical Chemistry, and Organic Chemistry, University of Huelva, Campus de El Carmen, s/n, E-21071 Huelva, Spain

[‡] Department of Chemical and Biological Engineering, Physical Chemistry, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

Experimental Section

1 was prepared in its open E form following the method by Rentzepis.[1,2] The ^{1}H NMR spectroscopic data of **1** coincide with the reported ones. The measurements were performed in air-equilibrated acetonitrile (spectroscopic quality) solution at room temperature.

The absorption measurements were done using a CARY 4000 UV/vis spectrometer. For the emission measurements, a SPEX Fluorolog τ2 was used. The UV and the visible light used for the photoisomerizations in the spectral measurements were generated by a UVP hand-held UV lamp (365 nm, model UVGL-25, 1.5 mW/cm^2) and a 500 W Xe-lamp, respectively. The Xe-lamp light was filtered by a long-pass glass filter ($A < 1$ at $\lambda > 540$ nm). The resulting light power density on the sample was 1.4 W/cm^2. The photostationary state distribution was estimated by ^{1}H NMR measurements.

The laser used to generate the input signals for the D flip-flop was an Nd:YAG laser (Continuum Surelite II-10, fwhm 6 ns). For reasons of experimental convenience only one laser was used to provide both inputs (*In* and *Clock*), while Scheme 3 shows two separate lasers to facilitate the description of the experimental approach. The cuvette containing a solution of **1** (*ca*. 5×10^{-5} M) was irradiated with the Nd:YAG laser through a SHG and then a THG crystal. The wavelength selection was achieved by rotating the crystals into and out of the resonance angle. The input situation "only *In* on" was generated by passing the first harmonic of the laser (1064 nm) through the two nonlinear crystals with the SHG and the THG crystals tuned off-resonance. The "only *Clock* on" situation was generated by tuning the SHG crystal in-resonance (532 nm) and the THG crystal off-resonance. When both crystals were in-resonance, 355 nm UV light was generated by the THG crystal, representing "both inputs on". Residual 1064 nm and 532 nm light after the THG crystal was not filtered off before passing the sample. This

is reflected in an incomplete conversion of **1E** to **1C**, which however does not interfere with the purely binary nature of the D-flip flop function. The irradiation powers and times employed were: 1064 nm (420 mW average power at 10 Hz for 45 s), 532 nm (30 mW average power at 10 Hz for 45 s), and 355 nm (18 mW average power at 10 Hz for 45 s). Had two lasers been available, crystal tuning could have been avoided. Various alternative setups, such as using a single laser and controlling the wavelength reaching the THG and sample with bandpass filters, or using a single laser with a beam splitter and electronically switched shutters, can be envisioned.

References

(1) Liang, Y. C.; Dvornikov, A. S.; Rentzepis, P. M. *Res. Chem. Intermed.* **1998**, *24*, 905-914.

(2) Liang, Y.; Dvornikov, A. S.; Rentzepis, P. M. *J. Mater. Chem.* **2000**, *10*, 2477-2482.