

Azobenzene photoisomerization quantum yields in methanol redetermined

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Supplementary information

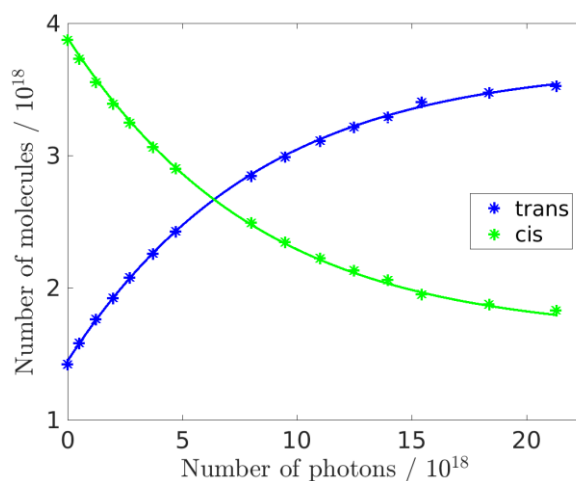


Figure S1: Calculated number of *trans*- and *cis*-azobenzene molecules during irradiation with fitted dependencies.

| Wavelength / nm | Calculated ratio of <i>c (trans)/c(cis)</i> in photostationary state | Experimental ratio of <i>c (trans)/c (cis)</i> approaching the photostationary state |
|-----------------|--|--|
| 280 | 0.716 | 0.875 |
| 313 | 4.56 | 4.58 |
| 334 | 18.4 | 16.3 |
| 405 | 0.194 | 0.229 |
| 436 | 0.233 | 0.274 |

Table S1: Calculated and experimental ratios of *trans*- and *cis*-azobenzene concentration

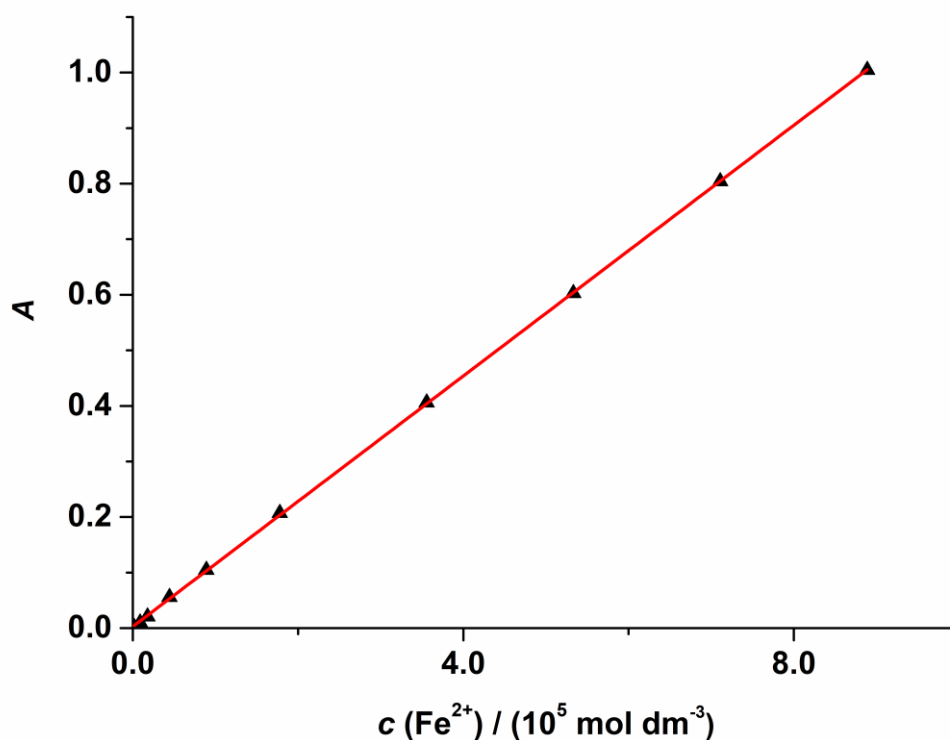


Figure S2: Calibration curve for ferrioxalate; dependence of the absorbance of tris(1,10-phenanthroline)iron(II) complex on concentration of Fe^{2+} .

Attached Matlab functions

1. photoheat.m

The function makes a fit of the evolution of concentrations of the substances A and B and calculates the quantum yields of the photochemical reactions $A \rightarrow B$ and $B \rightarrow A$. The substance can isomerize between two forms $A \leftrightarrow B$ by both photochemical and thermal reactions. The function determines the value and confidence intervals of both quantum yields and the total concentration of the substance (at the beginning of irradiation).

2. photoheat_input_data.m

All the input data are loaded by this function.

3. effectiveepsilon.m

The function calculates effective absorption coefficients of the irradiation source in respect with the measured absorbances.

4. resampling.m

The function resamples the spectra to facilitate the mathematical treatment of data not measured at identical wavelengths by applying linear interpolation.

5. process_ftA.m

Calculates the evolution of the concentrations of A and B that can be isomerized photochemically and thermally.

6. process_sum_of_squares_ftA.m

Calculates the sum of squares of differences between concentrations of A determined from the absorption spectra and those calculated from the model (eq. 5).

7. process_sum_of_squares_ftB.m

Calculates the sum of squares of differences between measured and calculated concentrations of the substance A. This function is used only when the total A+B concentration is fitted.

Attached azobenzene molar absorption coefficients

1. epsilon.dat

The values of the molar absorption coefficients of *trans*- and *cis*-azobenzene (second and third column, respectively) associated with the wavelengths given in the first column.

Attached example of measured data

1. concentrations.dat

The file contains the input information for quantum yields calculation, namely, times elapsed between measurements of absorbances in seconds (first column), number of photons incident on the cuvette (second column) and molar concentrations of the isomers A and B (third and fourth columns, respectively). The first number in both the first and the second column should be zero.

2. irradiation_beam.txt

This file contains the irradiation beam profile; the first column represents wavelengths, the second column represents the intensity at the given wavelength.

3. times.txt

The first column represents the irradiation period and the second column represents the period between measurements (both in s), including the time for measurement of the spectrum and that for manipulation of the sample.

4. readme.txt

The file contains tutoring information about the programs.