

Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry 2010

Supplementary information for

Naphthopyran dyes conjugated with fluorescent stilbazolium moieties in the pores of MCM 41 – photochromic and fluorescent properties

*Ingolf Kahle,^a Oliver Tröber,^b Hannes Richter,^b and Stefan Spange^{*a}*

Received (in XXX, XXX) Xth XXXXXXXXXX 20XX, Accepted Xth XXXXXXXXXX 20XX

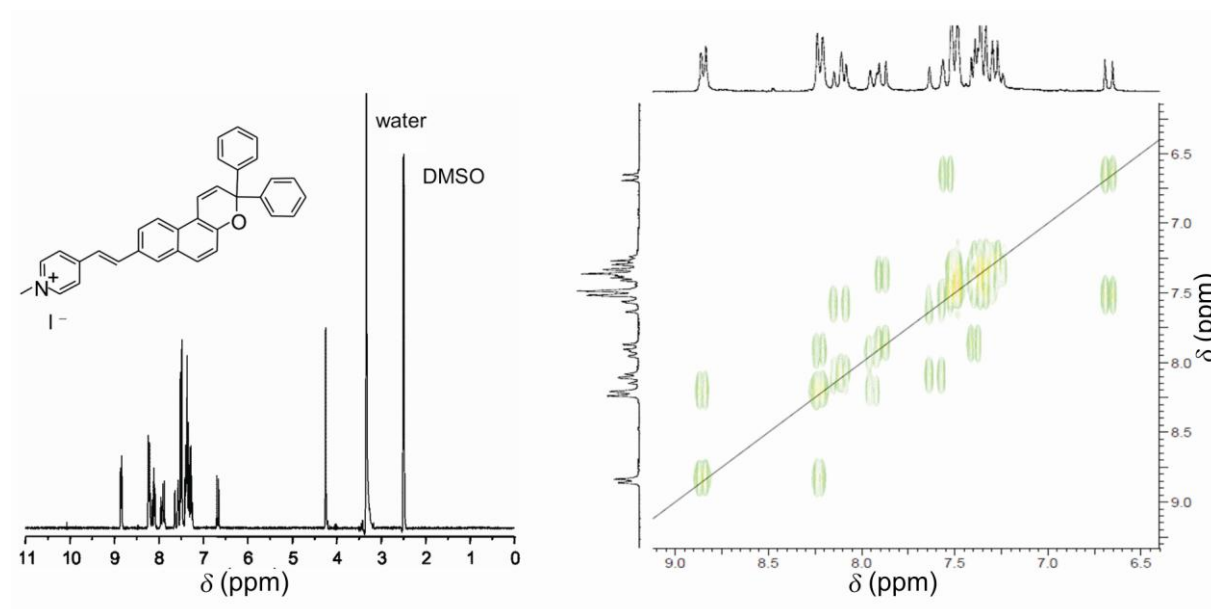
DOI: 10.1039/b000000x

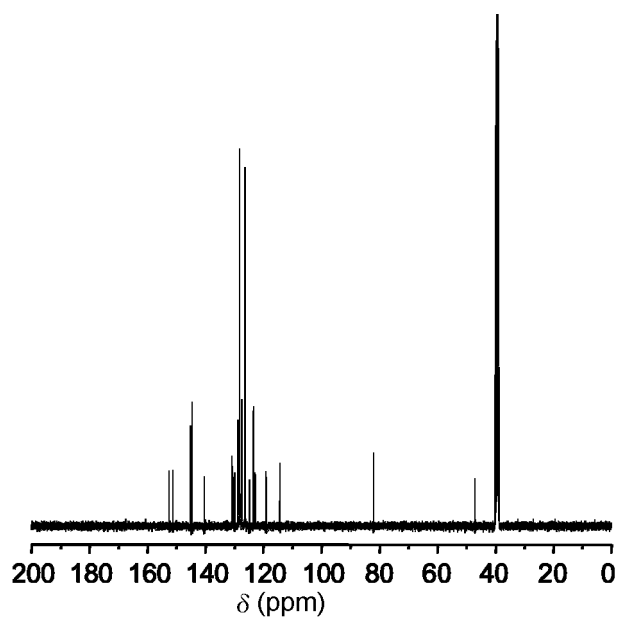
Content:

- NMR spectra (^1H -; ^{13}C ; HH-COSY) of compounds **3-6**
- UV/Vis spectroscopic investigation of photochromic host-guest systems
- Fluorescence measurements

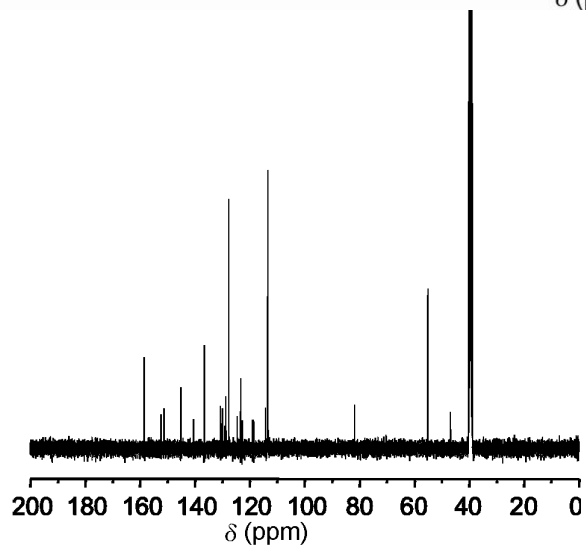
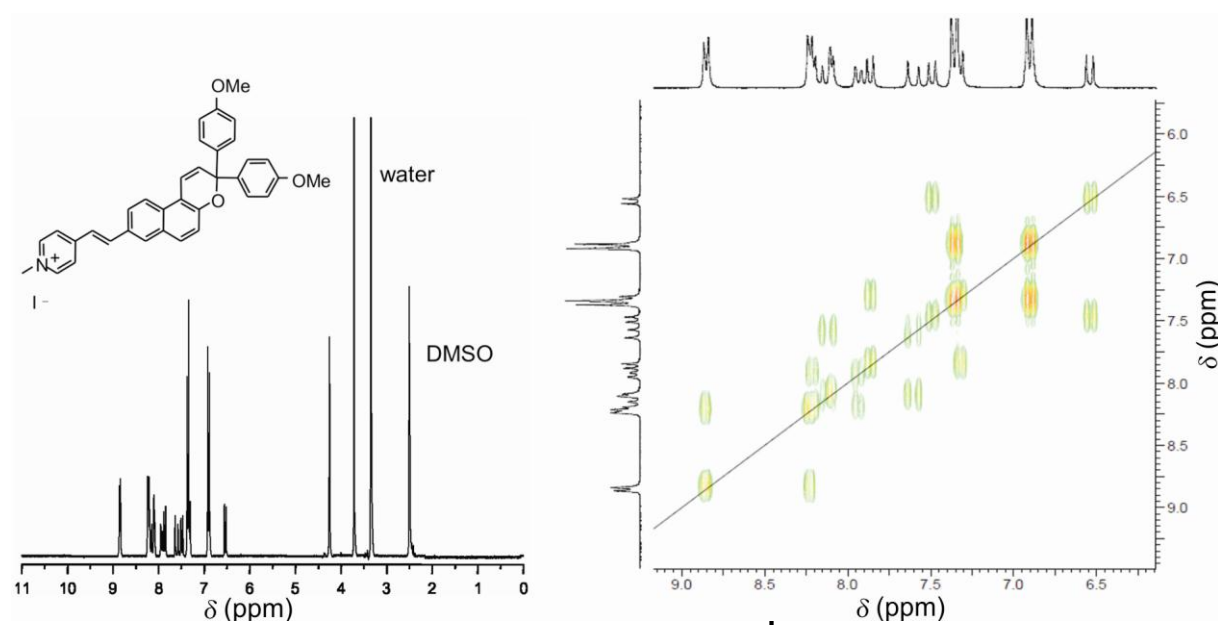
NMR spectra (^1H -; ^{13}C -; HH-COSY-) of compounds 3-6

*1-Methyl-(4-(3',3'-diphenyl-[3H]-naphtho[2,1-b]pyran-8'-yl)-vinyl)pyridinium iodide (**3**)*

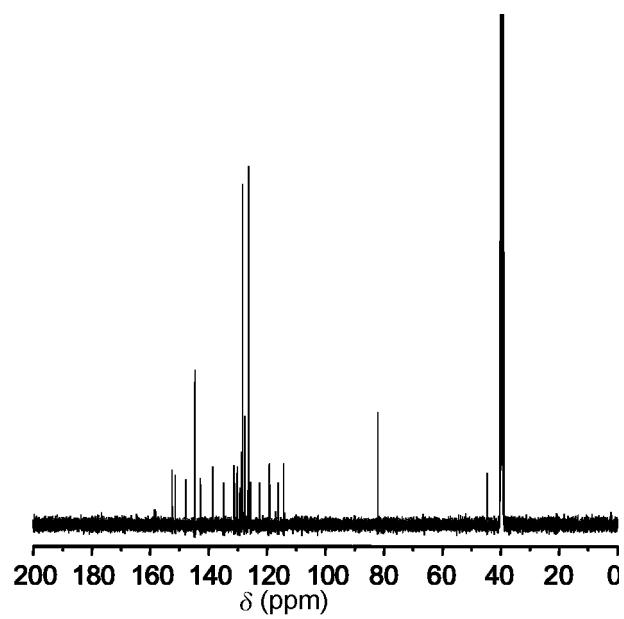
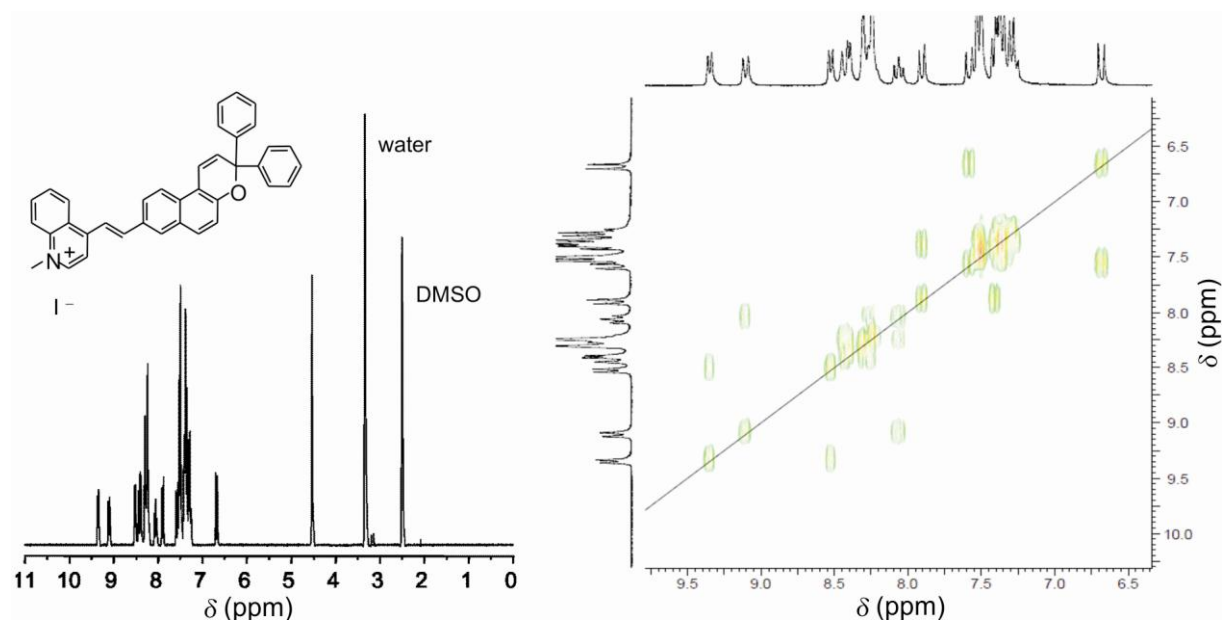




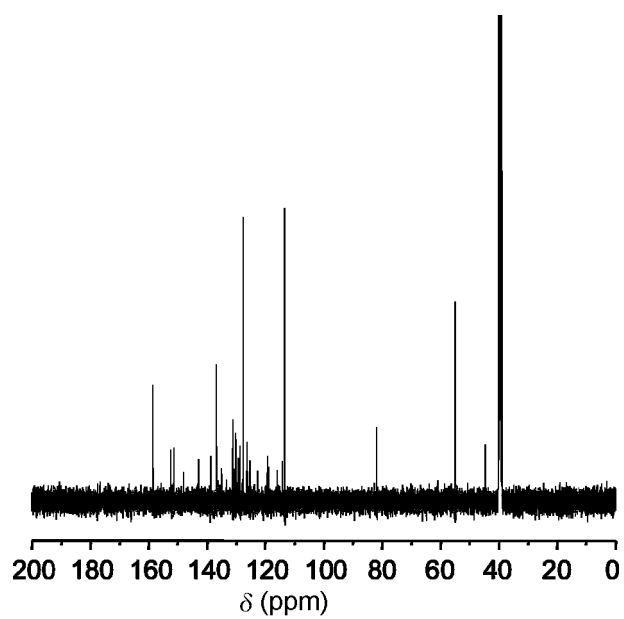
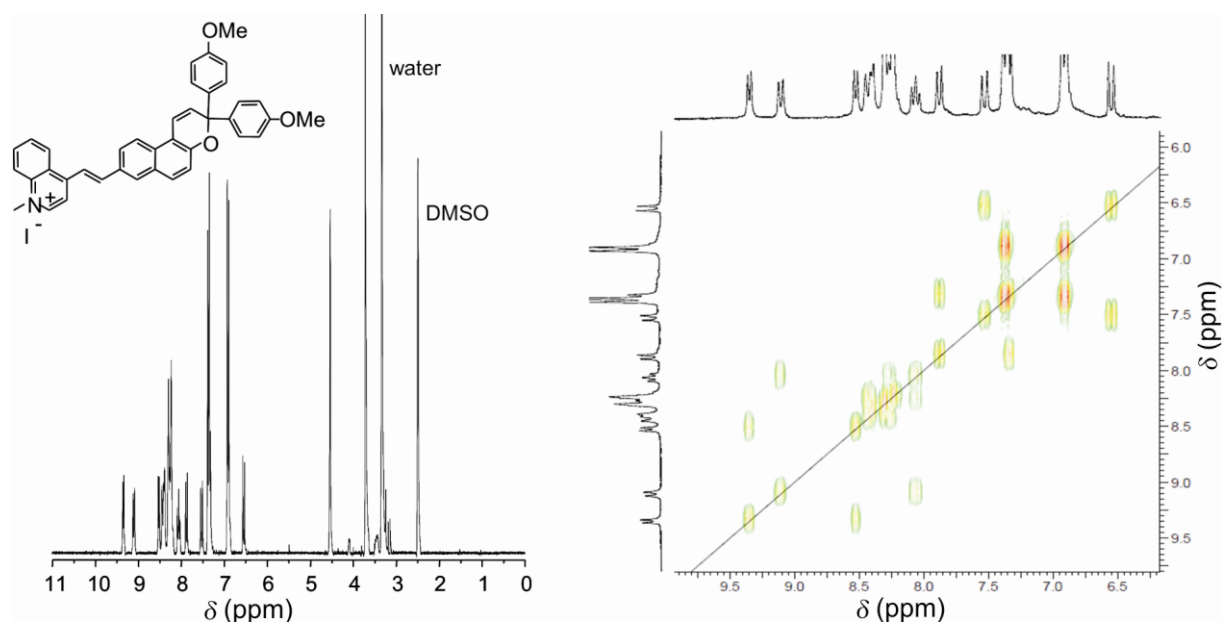
1-Methyl-(4-(3',3'-bis-(4-methoxyphenyl)-[3H]-naphtho[2,1-b]pyran-8'-yl)vinyl)pyridinium iodide (4)



1-Methyl-(4-(3',3'-diphenyl-[3H]-naphtho[2,1-b]pyran-8'-yl)-vinyl)pyrrolidinium iodide (5)

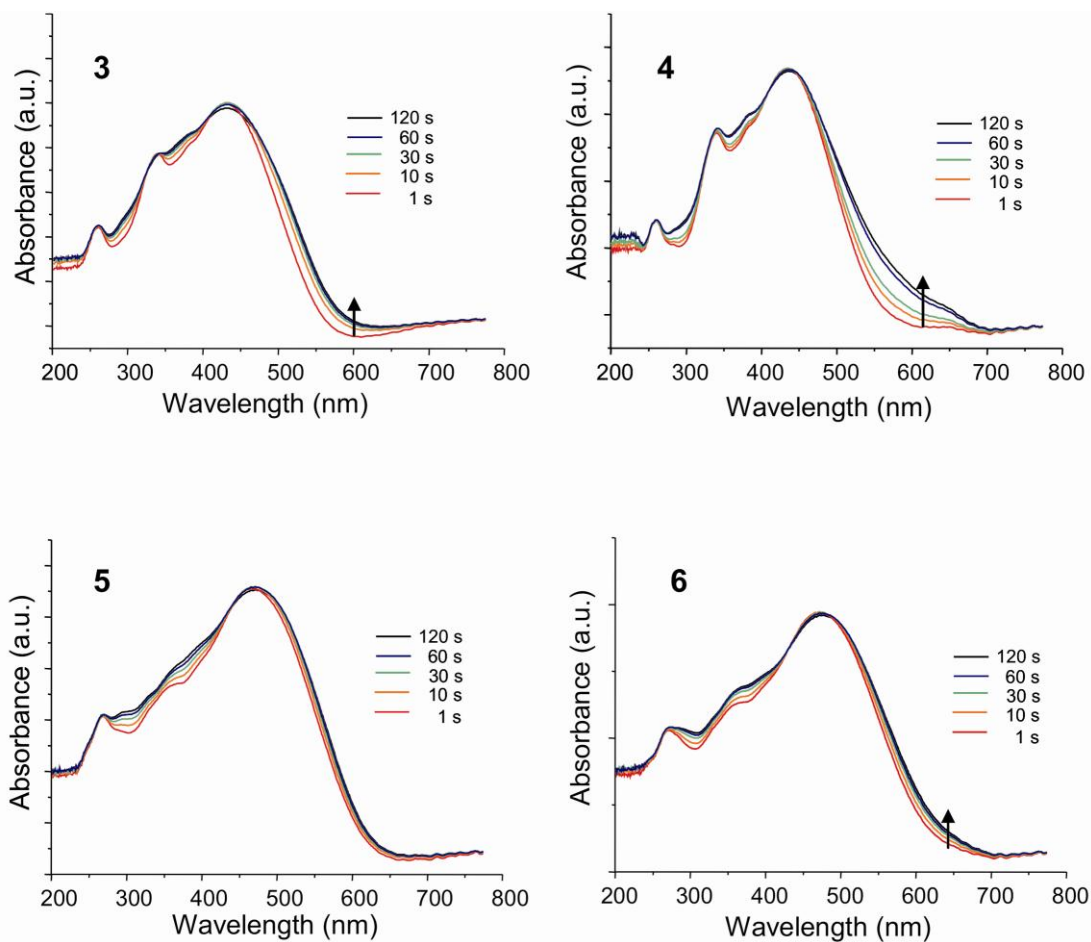


1-Methyl-(4-(3',3'-bis-(4-methoxyphenyl)l-[3H]-naphtho[2,1-b]pyran-8'-yl)vinyl)pyridinium iodide (6)

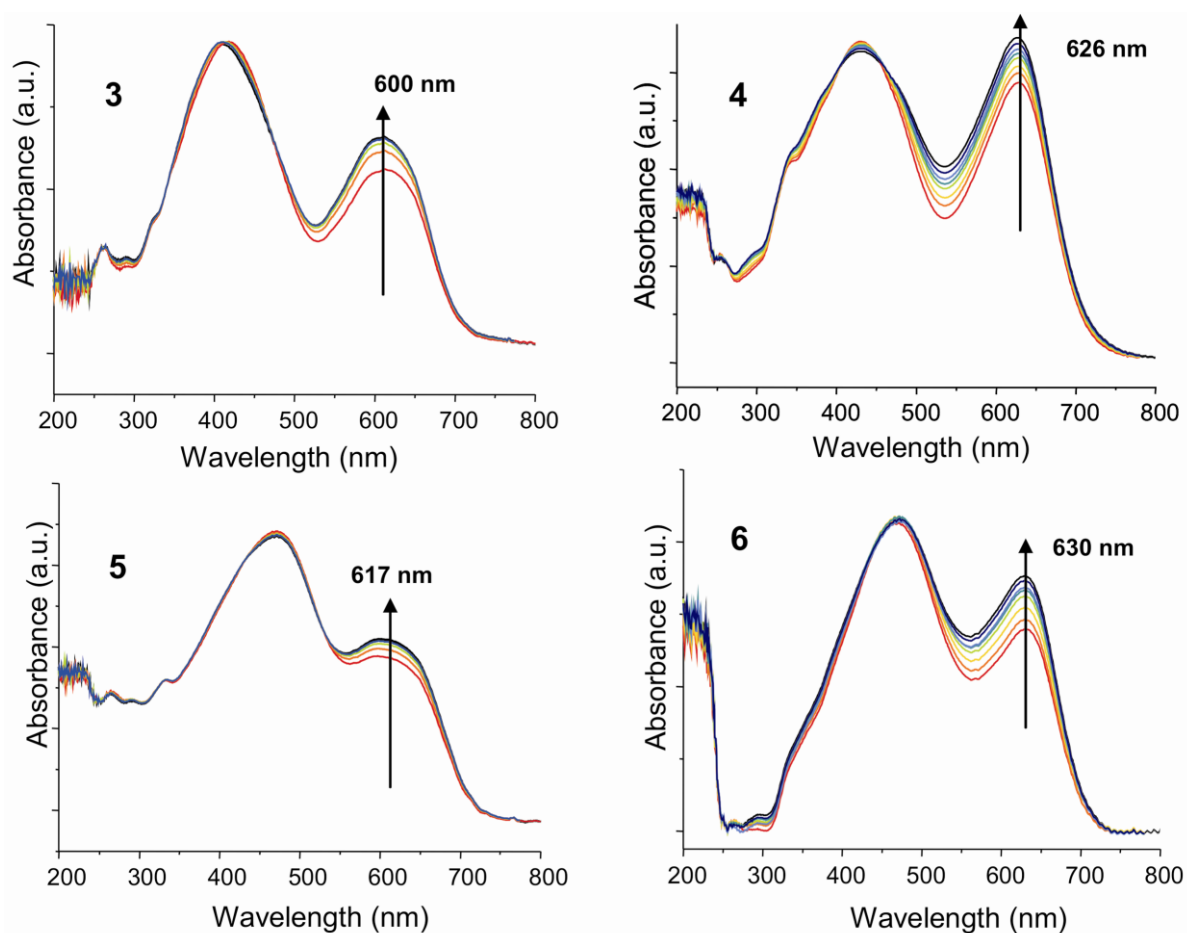


UV/Vis spectroscopic investigation of photochromic materials

The photochromic naphthopyran-conjugates **3-6** were incorporated into the pores of mesoporous surface-modified and non-modified MCM 41 particles by incipient wetness technique to prepare photochromic host-guest systems. These host-guest materials were investigated *via* UV/Vis spectroscopy while irradiating the samples simultaneously with UV-light (120 seconds at $\lambda = 350$ nm). Only a very weak photochromic response was observed for the fluorophore-conjugates **3**, **4** and **6** as they are either substituted by pyridinium units (**3** and **4**) which possess a much weaker electron withdrawing effect compared with that of a quinolinium moiety, or which are substituted with electron donating groups at the C-3 *geminal* aryl units (**4** and **6**). But photochromism is strongly increased for all compounds within the pores of non-modified MCM 41 particles. The spectral changes upon irradiation are shown below. Please note that each first spectrum was recorded 1 s after the samples have been irradiated.



UV/Vis spectra of compounds **3-6** in surface modified MCM 41 particles during UV irradiation for 120 s.



UV/Vis spectra of compounds **3-6** in non-modified MCM 41 particles during UV irradiation for 120 s.

Fluorescence measurements

The prepared photochromic host-guest systems showed a bright fluorescence, which decreases during illumination with UV-light. The following figure shows the changes of the emission maxima of each sample while excitation with 350 nm for a period of time and subsequent excitation at 500 nm for a several time period. Thereby, the black dots represent the measured intensity values and the red curves are the respective exponential fits which were used to calculate the half lives from table 2 in the main article.

