

Supporting Information

Study of the *E-Z* stilbene isomerisation in perchlorotriphenyl-methane (PTM) derivatives

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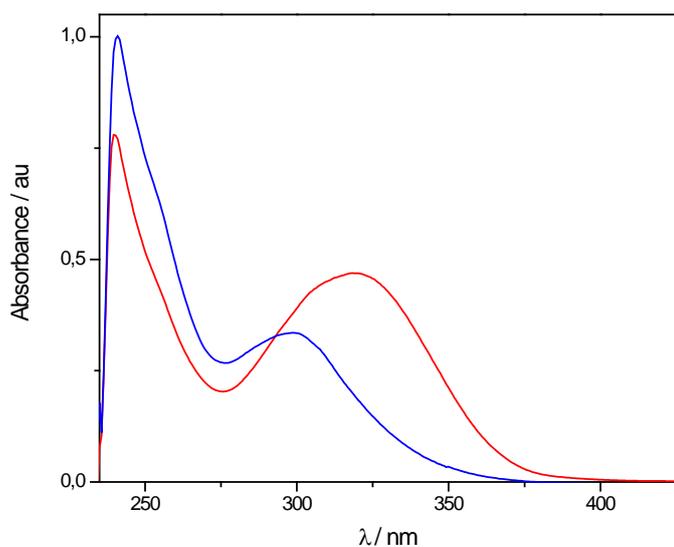


Figure S1. UV-vis spectrum in THF of *E-2*, in red, and of a *Z-2/E-2* mixture (99:1) in blue.

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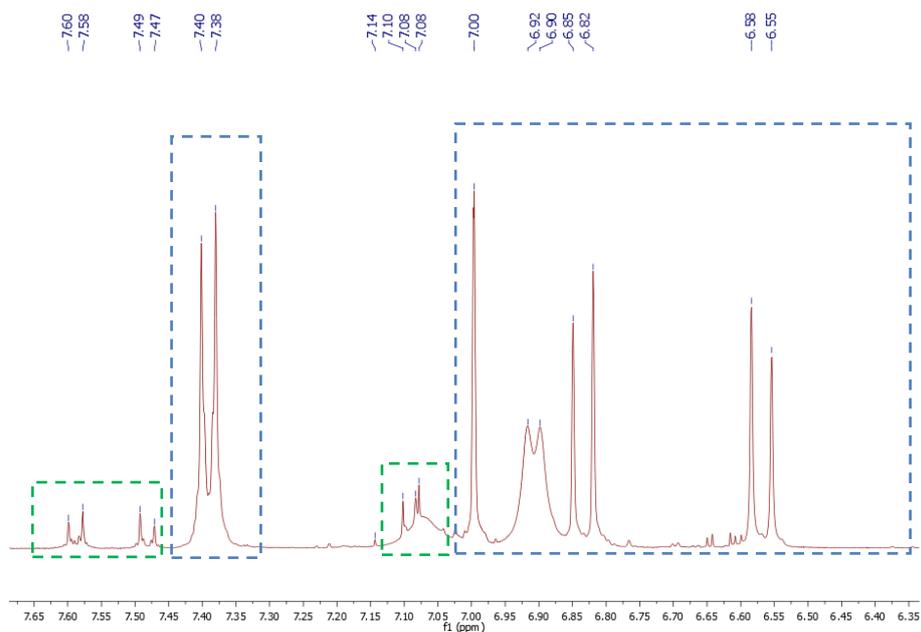
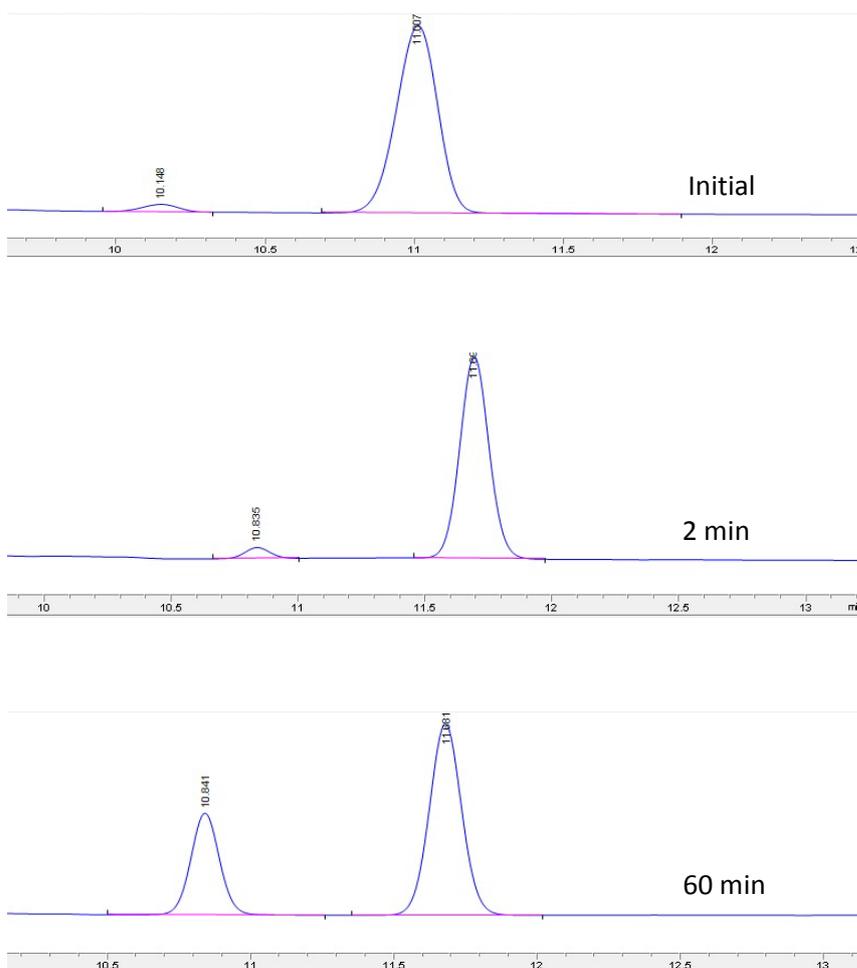


Figure S2. $^1\text{H-NMR}$ (400MHz) of compound **Z-2** in CD_2Cl_2 after irradiation during 450 min. *Z*-isomer signals are squared in blue, whereas the non-converted *E*-isomer signals are squared in gree



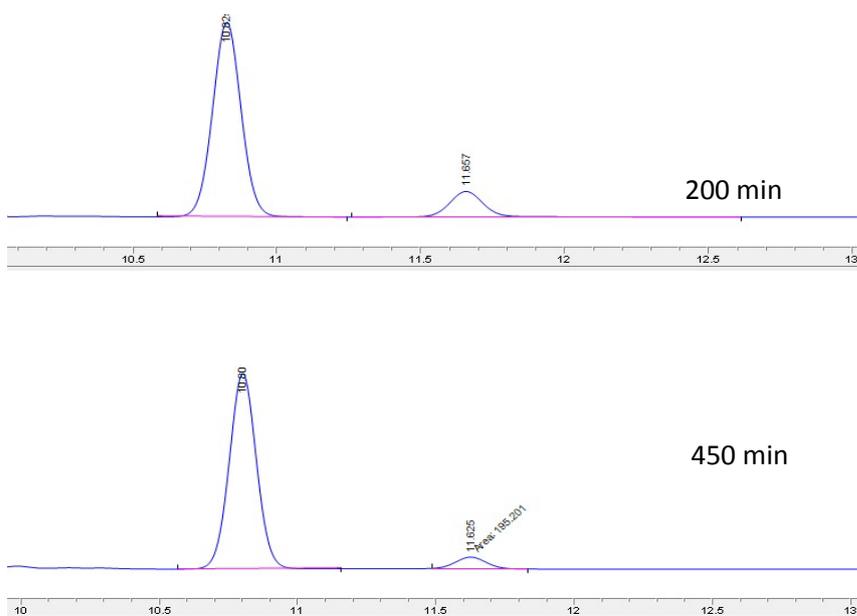


Figure S3. Time evolution of the isomerisation of compound **2** under illumination with a Hg(Xe) lamp. Experimental conditions: 3.2 mM solution of **2** in CHCl_3 was irradiated at 25 °C and aliquots were diluted and injected in HPLC, stationary phase C-18 reversed phase, mobile phase CHCl_3/ACN (20/80), 40 °C, UV detector with a fixed wavelength of 254 nm and a flow of 1ml/min.

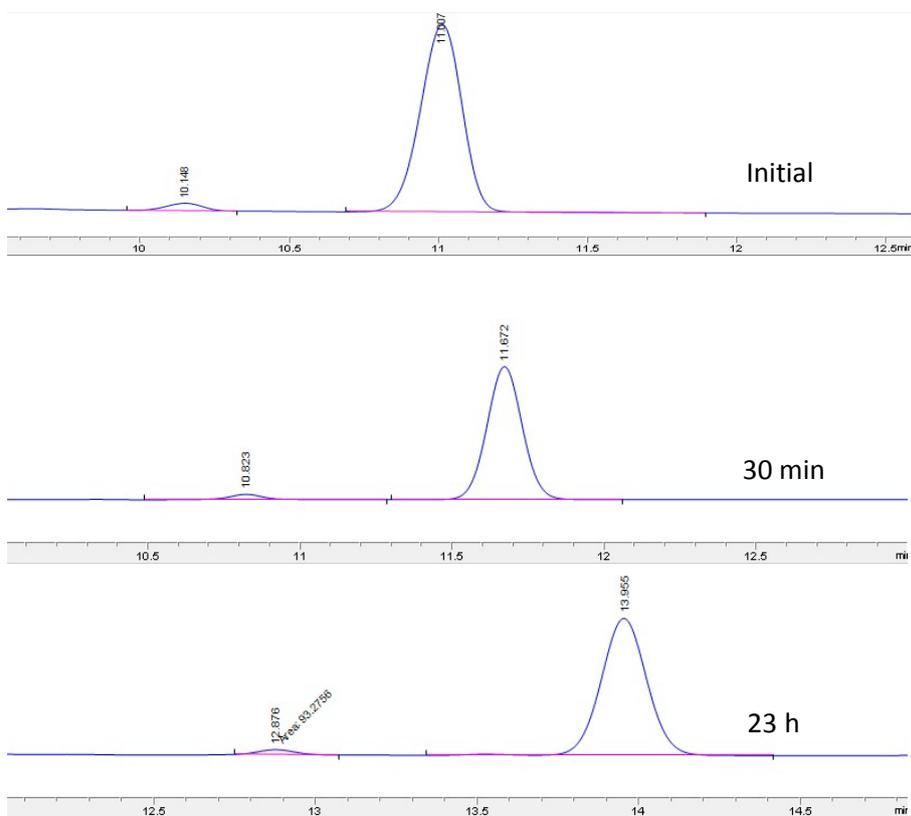


Figure S4. HPLC time monitoring of the effect of temperature on *E*-**2**. Experimental conditions: 0.067 mM solution of **2** in toluene was refluxed and aliquots were diluted and injected, stationary phase C-18 reversed phase, mobile phase CHCl_3/ACN (20/80), 40 °C, UV detector with a fixed wavelength of 254 nm and a flow of 1ml/min.

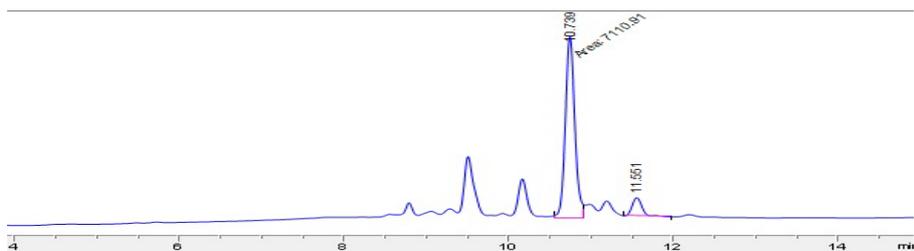
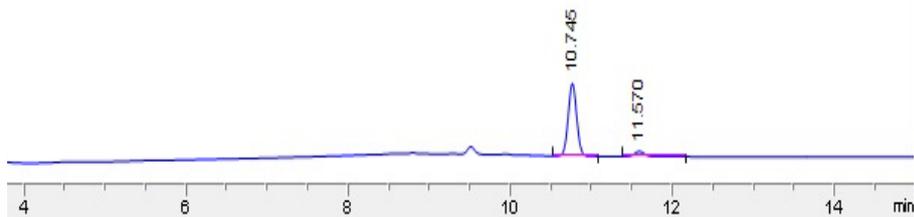
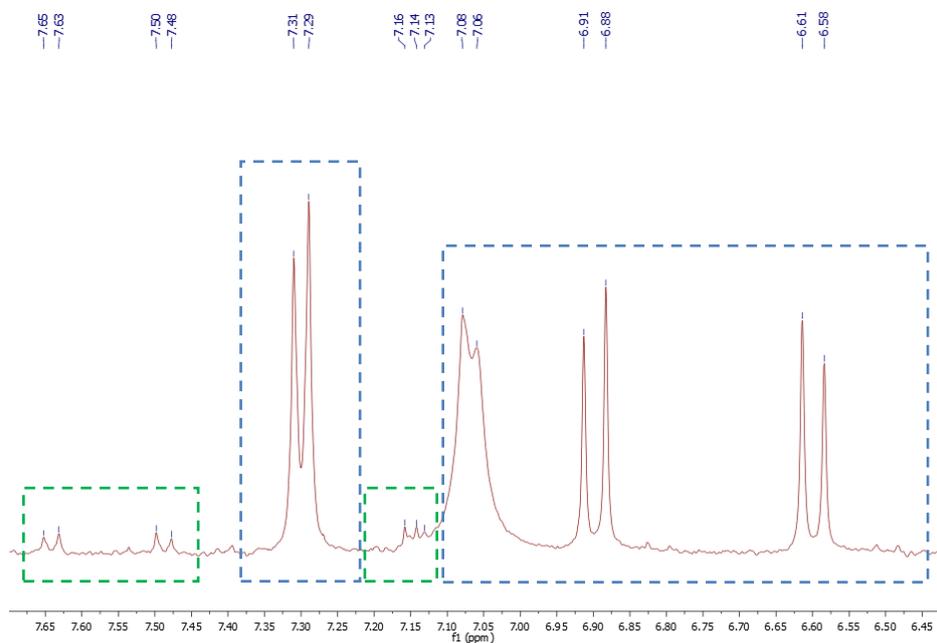


Figure S5. HPLC time monitoring of the isomerization trial catalyzed by I_2 of *Z*-2. Experimental conditions: 0.022 mM solution of the mixture obtained after 450 min illumination of *E*-2 in toluene, with 0.03 equivalents of I_2 , was refluxed and aliquots were washed with sodium sulfite, diluted and injected, stationary phase C-18 reversed phase, mobile phase $CHCl_3/ACN$ (20/80), 40 °C, UV detector with a fixed wavelength of 254 nm and a flow of 1ml/min.



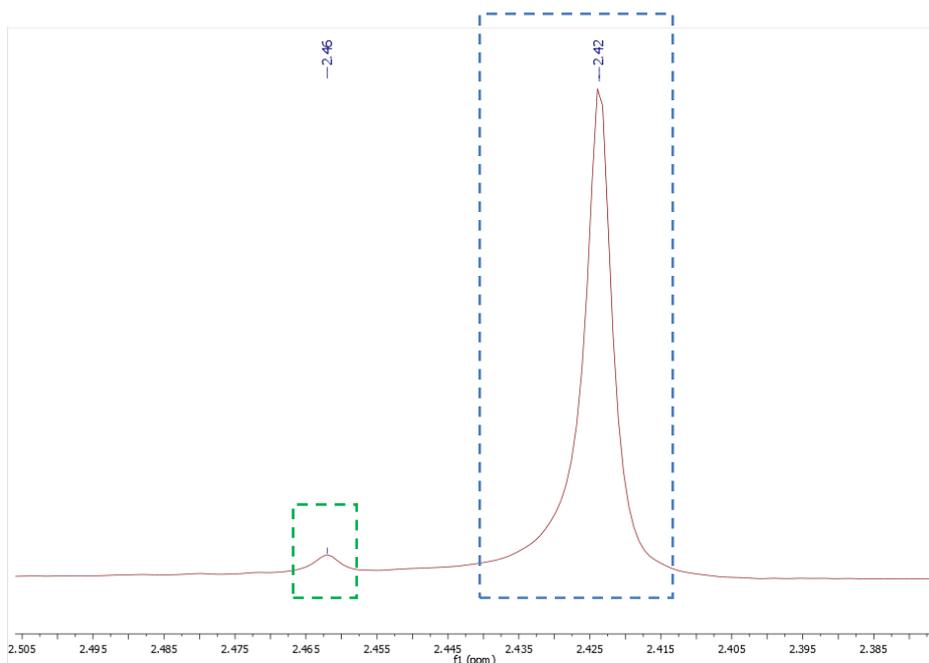


Figure S6. $^1\text{H-NMR}$ (400MHz) of the *Z*-1 in CD_2Cl_2 after irradiation during 145 minutes. *Z*-isomer signals are squared in blue, whereas the non-converted *E*-isomer signals are squared in green.

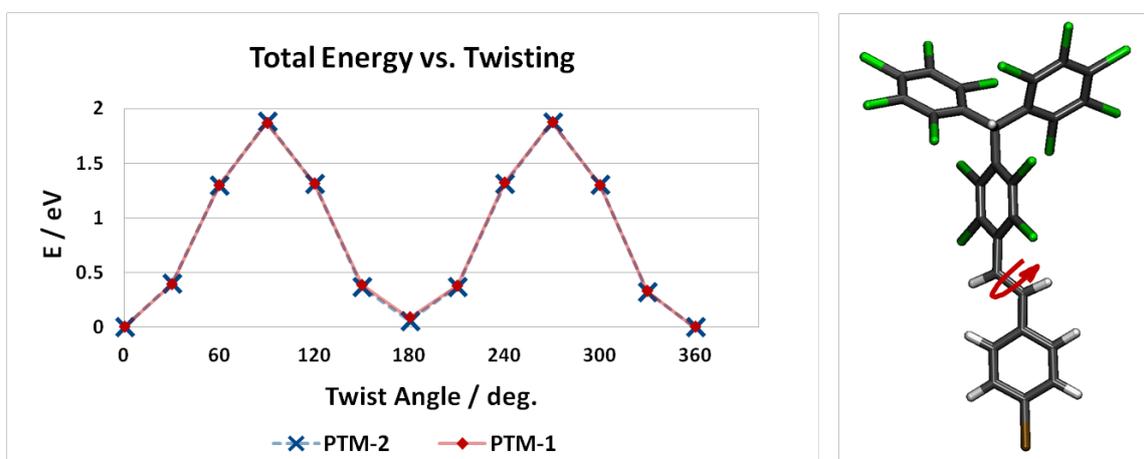


Figure S7. Manual twisting of the $\text{C}=\text{C}$ bond (see red arrow on **2** structure) by means of DFT constrained optimizations using the PBE0 hybrid functional and a 6-311-G++ basis set as implemented in the Gaussian09 code. The plotted energies are referenced to the most stable conformation for each compound (i.e. *E*-1 and *E*-2, respectively).

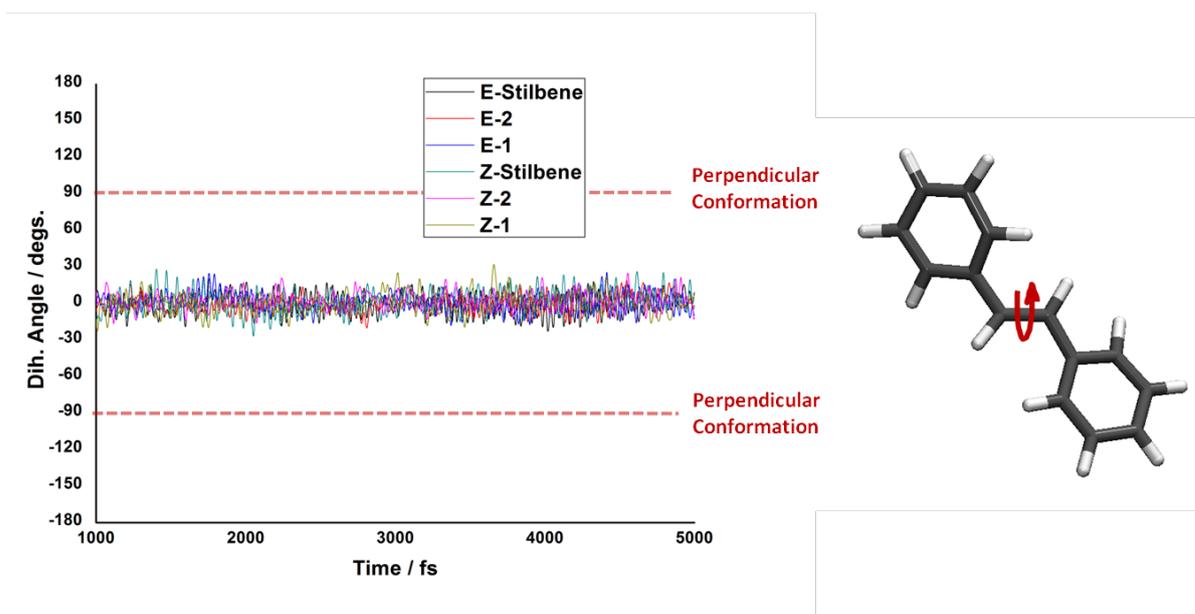


Figure S8. Variation of the dihedral angle of the central vinylene unit (C=C bond, see red arrow on stilbene structure) during 4 ps of a molecular dynamics simulation at 450K for our three studied compounds (**1**, **2** and stilbene) in each conformation (*E* and *Z*). Such calculations were performed using the PBE0 hybrid functional, the Bussi-Donadio-Parrinello thermostat and a light numerical basis set as implemented in the FHI-AIMS code. Red dashed lines point to the hypothetical perpendicular conformations for comparison.