SUPPORTING INFORMATION

Using potassium bromide pellets and optical spectroscopy to assess the photodimerization of two *trans*-(Trifluoromethyl)-cinnamic acid compounds.

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Contents:

Materials and methods

FTIR spectra of *trans*-3-(trifluoromethyl) cinnamic acid (3-tfmca) and *trans*-4-(trifluoromethyl) cinnamic acid (4-tfmca) were recorded on a Perkin Elmer Spectrum Two spectrophotometer in mineral oil (often called Nujol) and potassium bromide (KBr) pellet in the wavenumber region of 4000-400 cm^{-1} with a resolution of 1.0 cm^{-1}. Nujol was purchased from Merk/Sigma Aldrich with product number M3516. It has the CAS No.: 8042-47-5. The thickness of the pellet was around 0.5 mm and the optical path length of the Nujol sample was 0.2 mm defined by a teflon spacer. The powder sample was dispersed in the Nujol as good as possible forming a fairly homogeneous suspension. However, it was difficult to keep a constant concentration in the Nujol case since the powder sample was slowly drifting to the bottom of the cuvette during the measurement.

Thermogravimetric analyses were conducted on HITACHI TG/DTA 7300 at a heating rate of 10 °C/min. Approximately 8 mg of irradiated powders were taken as a sample.

Table T1. The crystal data of 3-tfmca, 4-tfmca, and partially photodimerized 4-tfmca after 8 hours of irradiation.

	3-tfmca	**4-tfmca**	**4-tfmca-8h**
Formula	$C_{10}H_7F_3O_2$	$C_{10}H_7F_3O_2$	$C_{20}H_{14}F_6O_4$
Formula weight	216.16	216.16	432.31
Temperature/K	293(2)	293(2)	293(2)
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	$P\bar{1}$	$P\bar{1}$
a, Å	14.3911(9)	7.8672(5)	7.8930(5)
b, Å	4.9722(3)	7.9953(6)	8.2222(6)
c, Å	13.1778(8)	14.9972(11)	14.6037(12)
α, °	90	91.368(6)	89.860(6)
β, °	91.829(6)	93.753(5)	88.678(6)
γ, °	90	94.796(5)	82.349(6)
Volume, $Å^3$	942.46(10)	937.61(12)	939.06(12)
Z	4	4	2
ρ_{calc}, g/cm^3	1.523	1.531	1.529
μ, mm^{-1}	0.144	0.145	0.144
F(000)	440.0	440.0	440.0
Measured reflections	9129	30088	14300
Independent reflections	1915	5732	3763
R(int)	0.0438	0.0293	0.0408
Goodness-of-fit on F^2	1.106	1.071	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0584, wR_2 = 0.1356	R_1 = 0.0498, wR_2 = 0.1529	R_1 = 0.0905, wR_2 = 0.2737
Final R indexes [all data]	R_1 = 0.0808, wR_2 = 0.1474	R_1 = 0.0757, wR_2 = 0.1710	R_1 = 0.1446, wR_2 = 0.3230
CCDC deposition number	2331099	2331642	2332753

Table T1 gives an overview of the single crystal data. It links the numbers of the structures published in the Cambridge Structural Database (CCDC) with the two compounds under investigation, 3-tfmca and 4-tfmca.

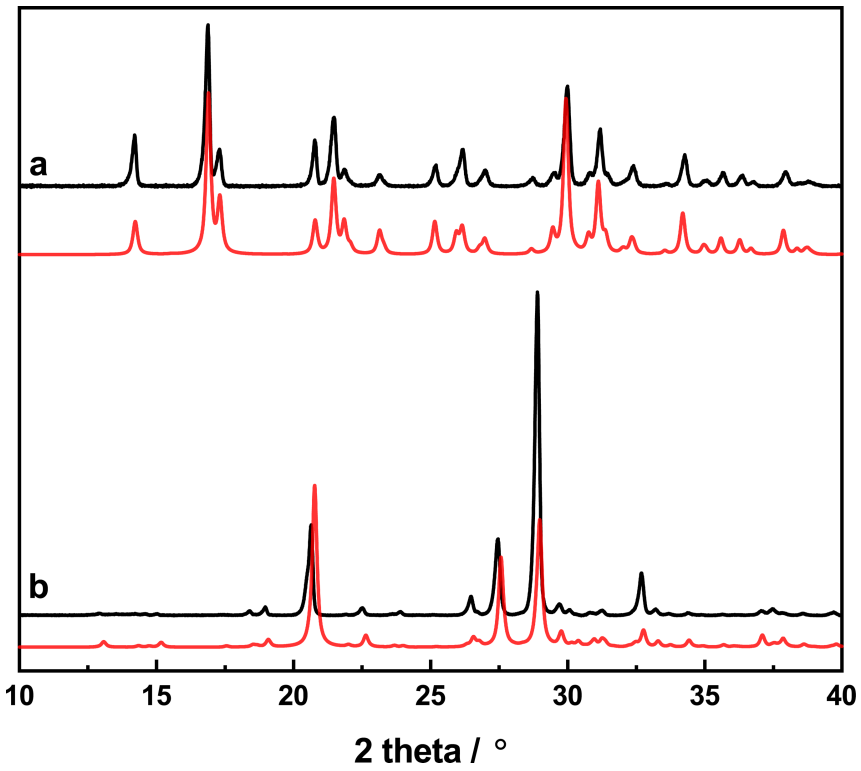

Figure S1. Experimental (black line) and calculated (red line) X-ray diffraction patterns for (a) 3-tfmca and (b) 4-tfmca.

Figure S1 is intended to link the powder data to the single crystal data. The measured powder patterns are compared with the ones calculated from the single crystal data using the software Mercury provided by the website of the Cambridge Crystallographic Data Centre (CCDC).

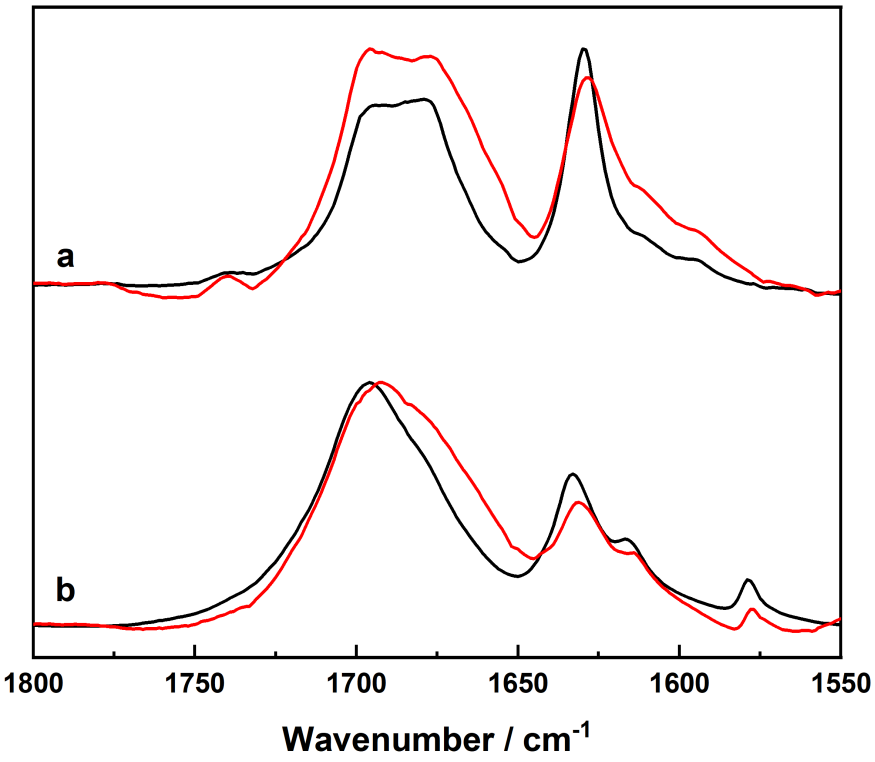

Figure S2. FTIR spectra of (a) 3-tfmca and (b) 4-tfmca recorded in KBr pellet (black line) and Nujol (red line).

Figure S2 shows the infrared absorption spectra of the 3-tfmca (part a) and the 4-tfmca (part b) compound measured in the potassium bromide pellet (black line) and in Nujol, in a red line. Good agreement between the infrared spectra in the two different environments, potassium bromide and Nujol shows that the residual pressure in the pellet does not change the vibrational structure of the molecules in it considerably. We attribute the observed changes more to the effects of the different dielectric constants of the two dispersants.

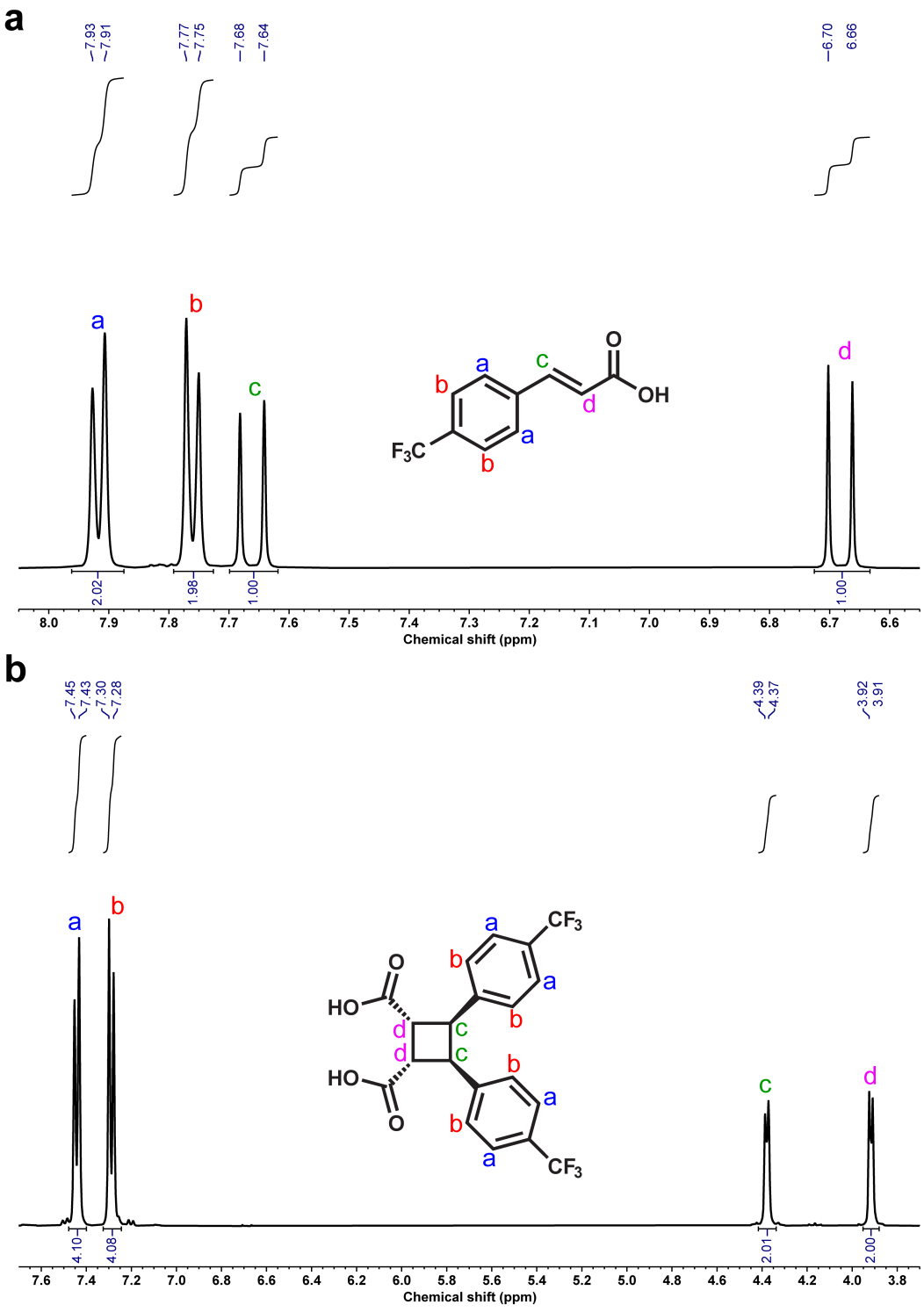

Figure S3. ^{1}H NMR spectra of (a) 4-tfmca and (b) sample irradiated with mercury xenon lamp for 480 mins.

Figure S3 illustrates the peak assignment of the NMR spectra of the (part a) pristine 4-tfmca powder and (part b) irradiated 4-tfmca powder. Basic data treatment processes such as phasing, baseline correction, chemical shift referencing, peak picking, and peak integration were performed with MestReNova *v14.2.1-27684* software.

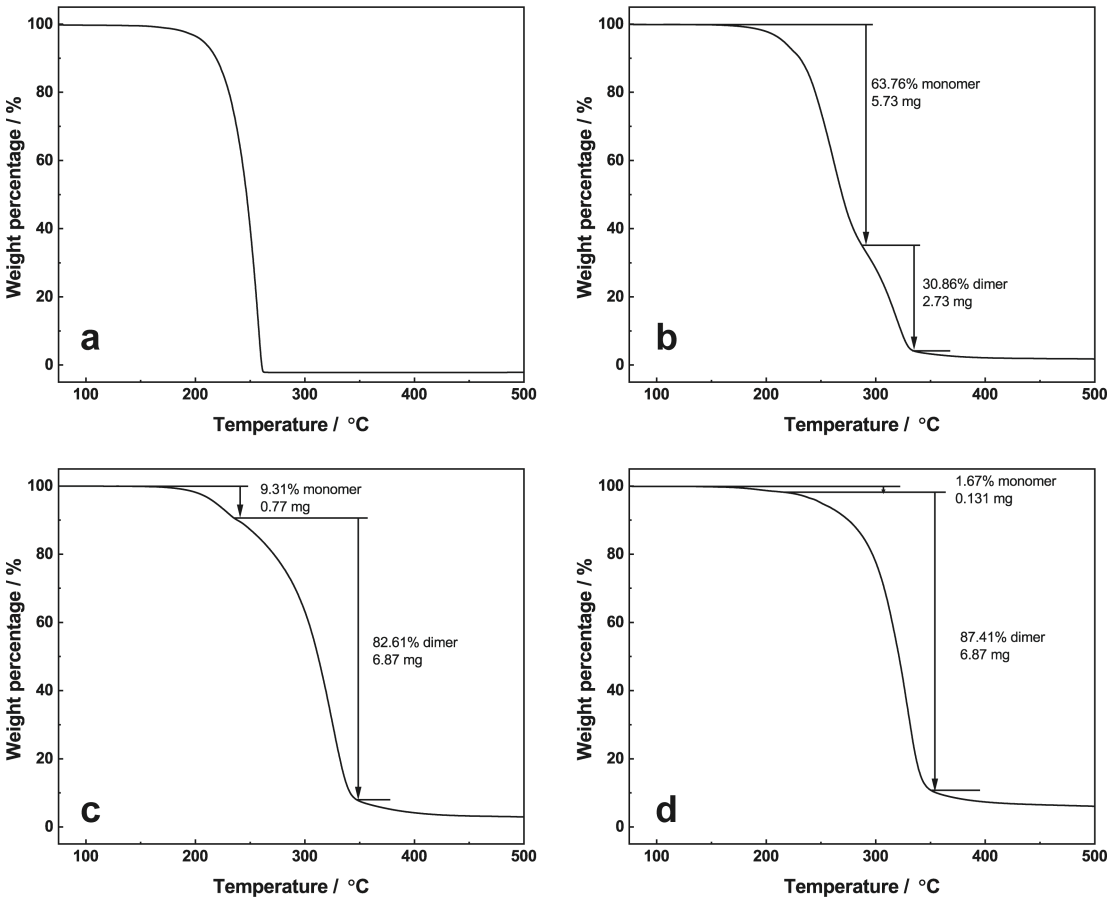

Figure S4. TG plots of (a) 4-tfmca and samples irradiated with mercury xenon lamp for (b) 180, (c) 360 and (d) 480 mins.

Figure S4 displays a series of thermogravimetric plots of 4-tfmca after UV irradiation (0, 180, 360, 480 mins) with each plot representing the mass loss % of the sample as a function of temperature, providing the estimate of the progress of the reaction, and to the conversion yield (in mass %). Because the decomposition of both reactant 4-tfmca and the product 4,4′-ditrifluoromethyl-β-truxinic acid is not clearly separated the conversion yields shown in the plots are only rough estimates.