

# Photochemical reactivity of a lamellar Lanthanum MOF

**Adonis Michaelides,<sup>\*a</sup> , Maria Aravia,<sup>a</sup> Michael G.  
Siskos<sup>\*a</sup> and Stavroula Skoulika<sup>\*a</sup>**

[vskoul@uoi.gr](mailto:vskoul@uoi.gr), [amihail@uoi.gr](mailto:amihail@uoi.gr), [msiskos@cc.uoi.gr](mailto:msiskos@cc.uoi.gr)

Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece

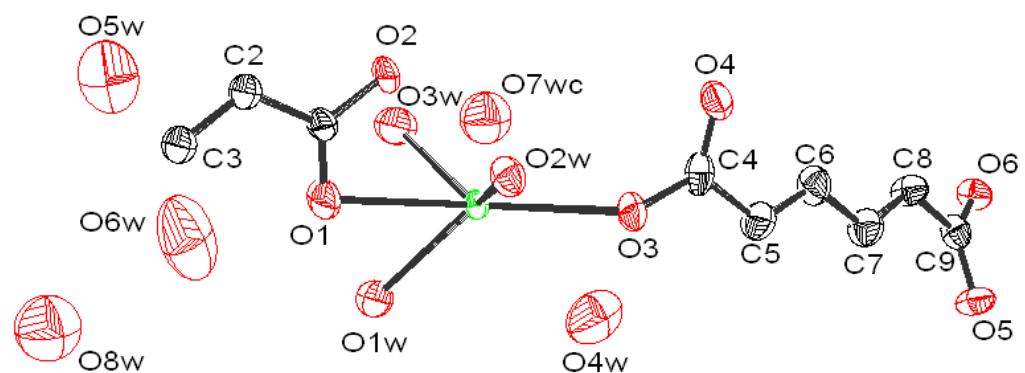


Figure S1. ORTEP drawing of the asymmetric unit of compound **1**.

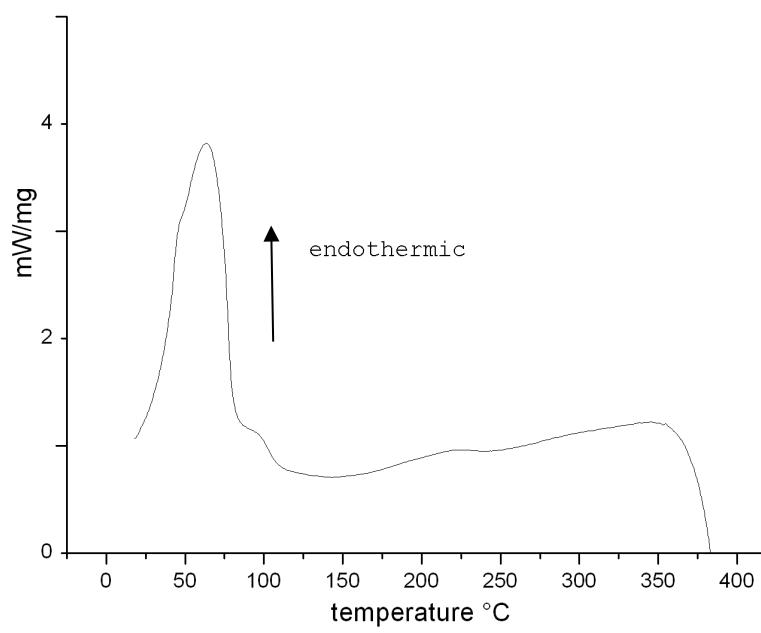
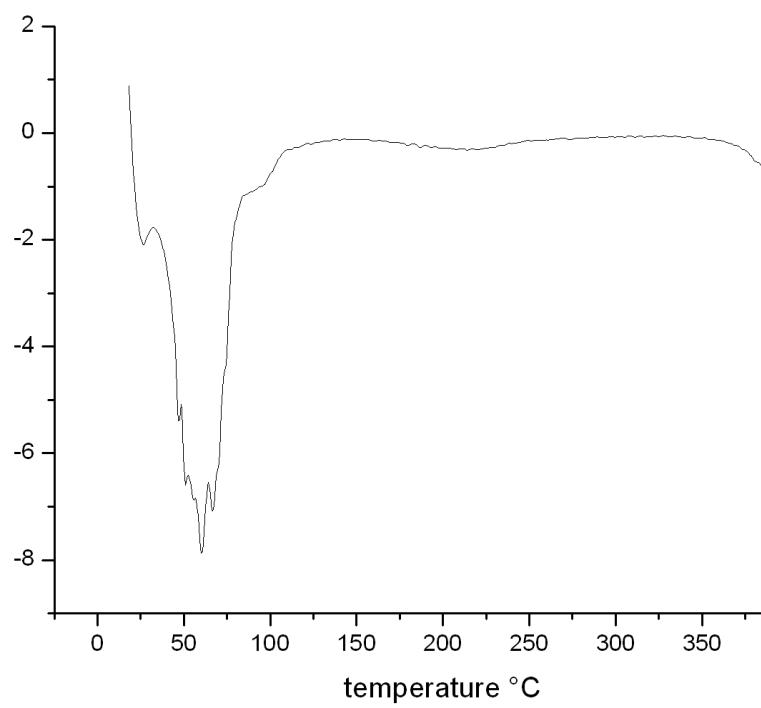
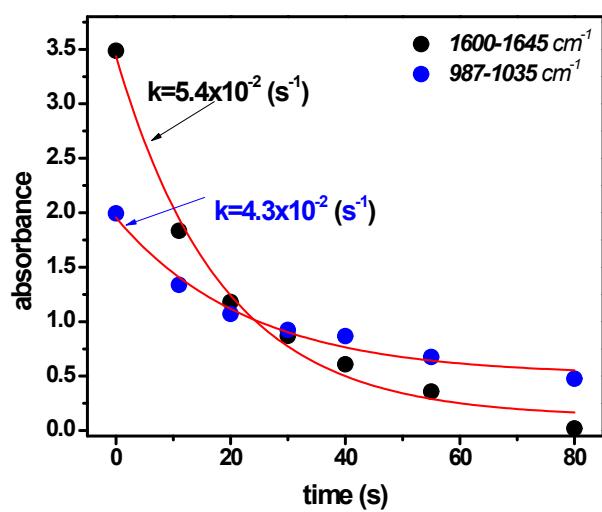
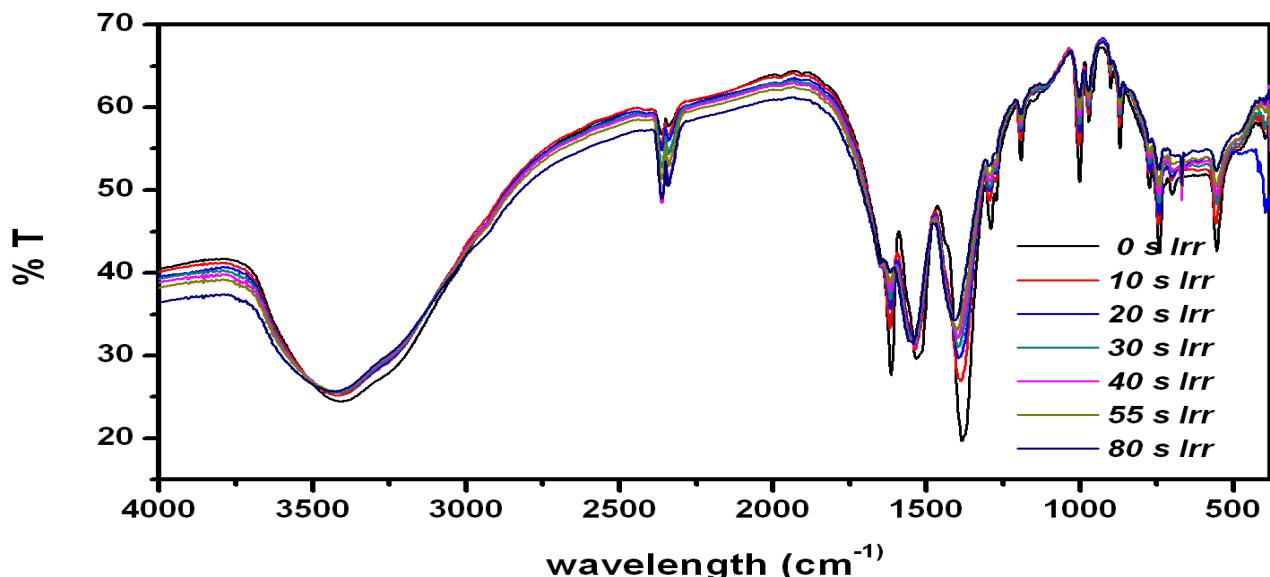
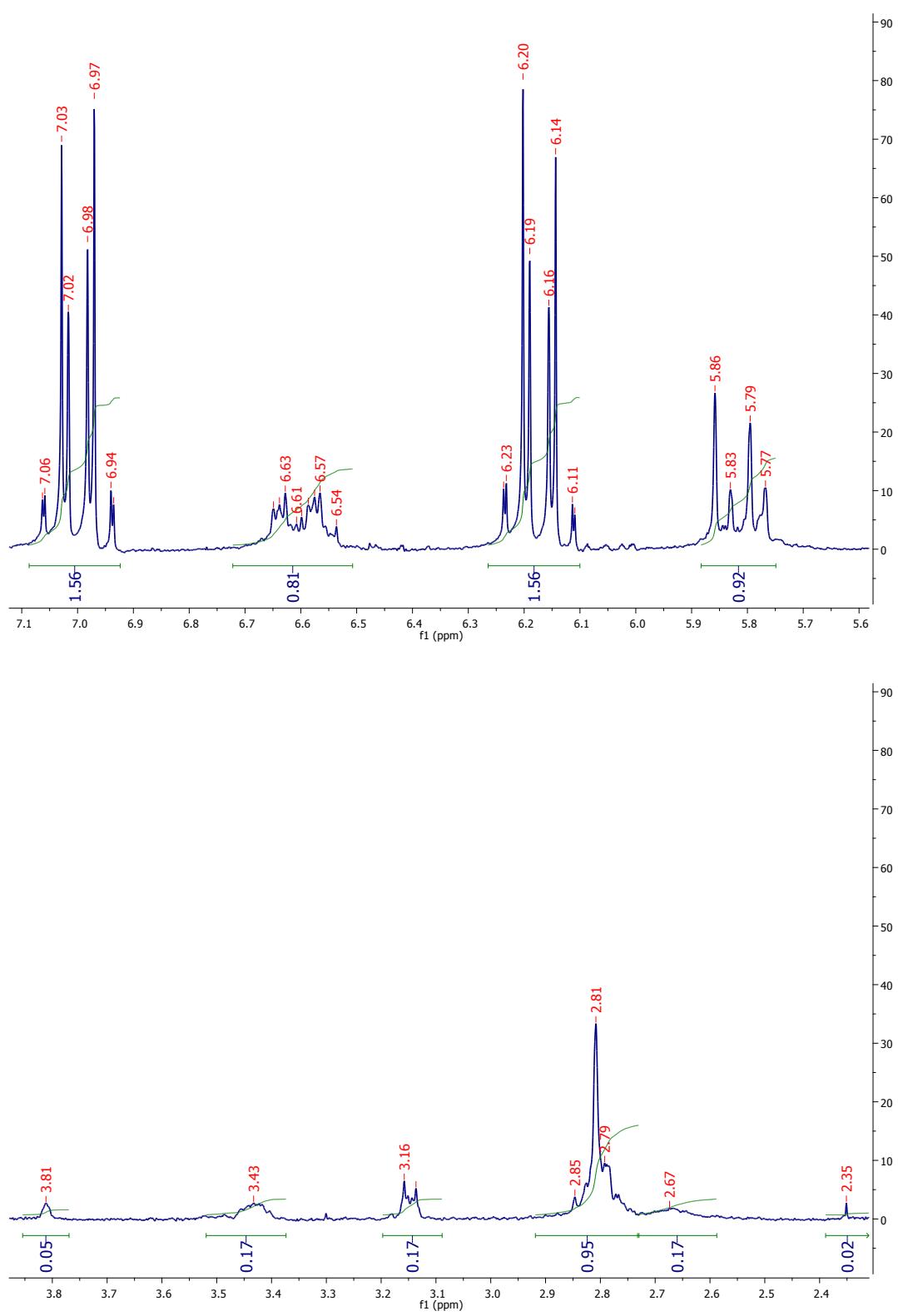


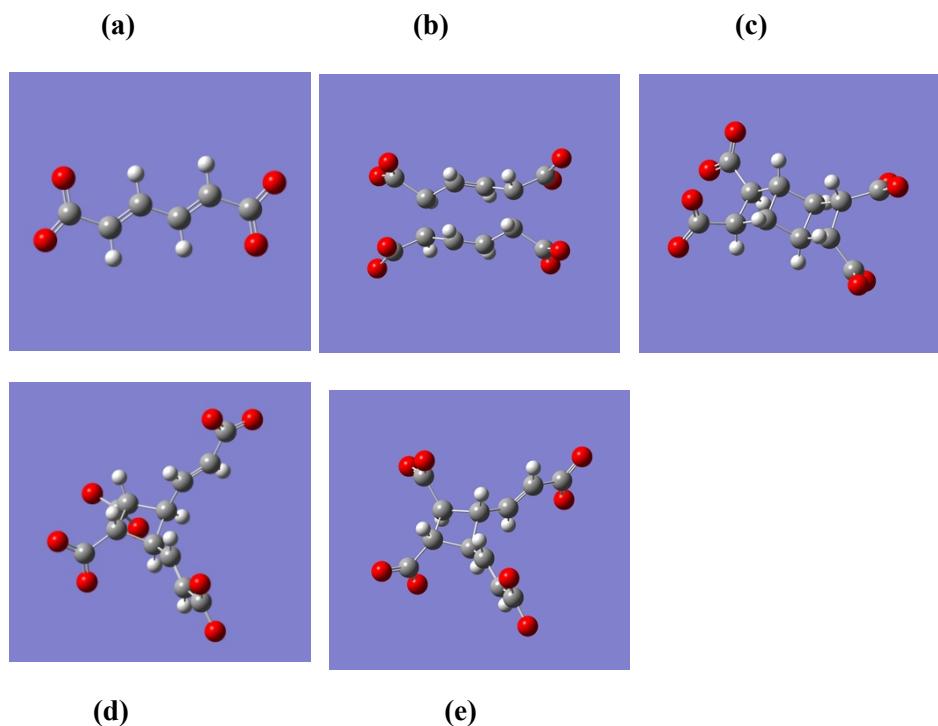
Figure S2. Top: DTG analysis of compound **1**. Bottom: DSC analysis of compound **1**.



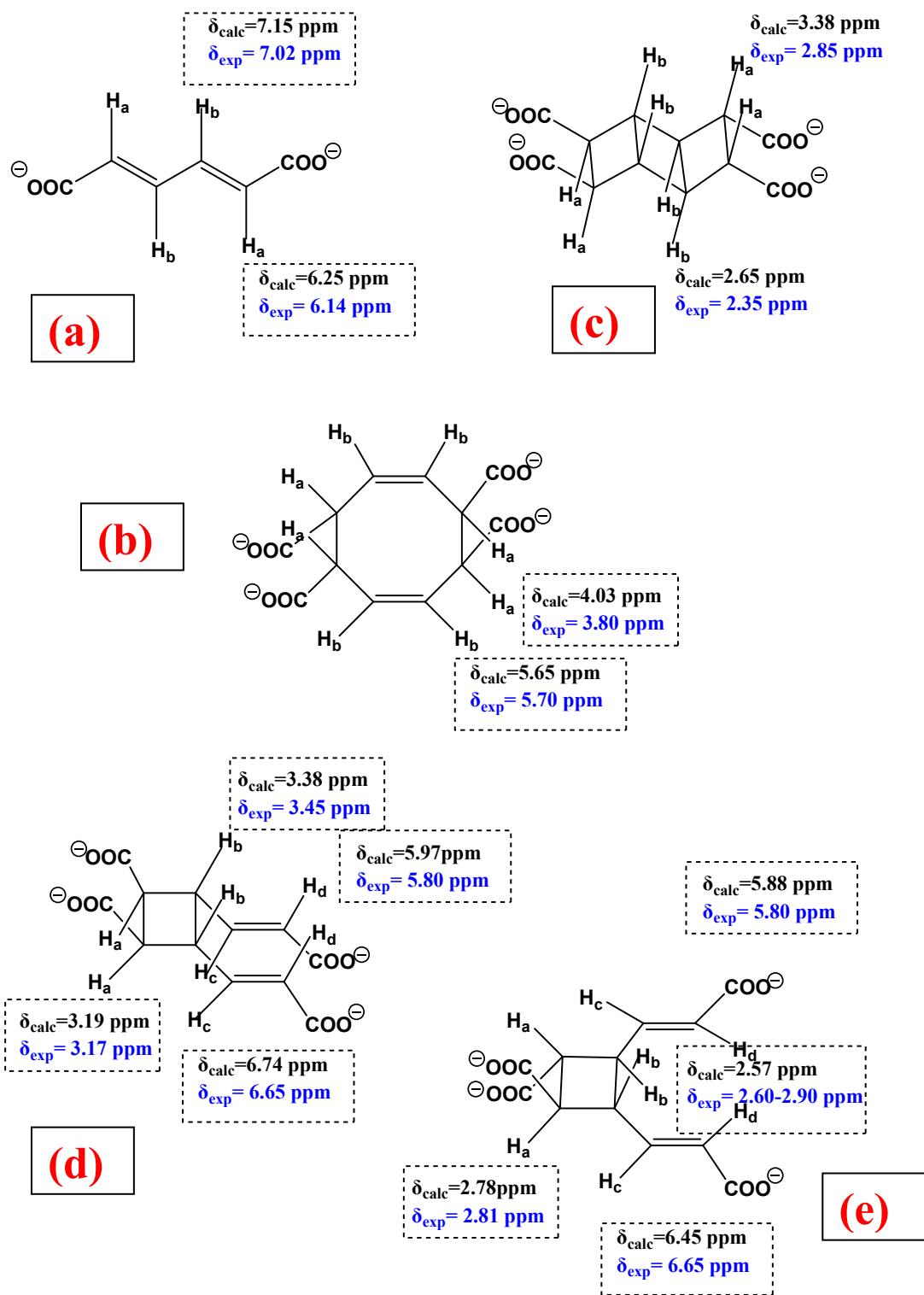
**Figure S3.** Top: IR spectrum of compound **1** as a function of irradiation time. Bottom: Absorbance in two spectral regions as a function of irradiation time with the corresponding calculated reaction constants for compound **1**.



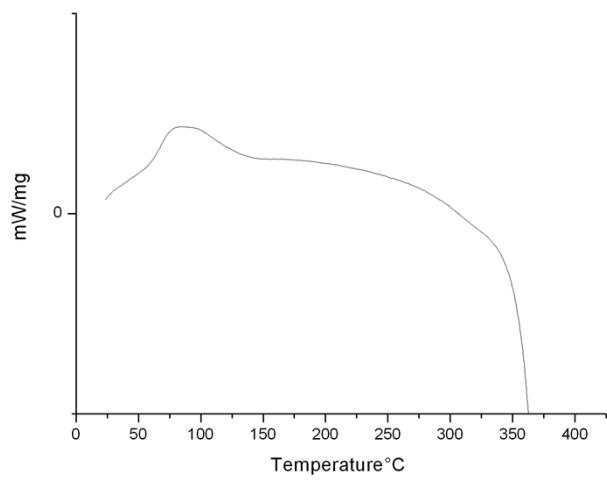
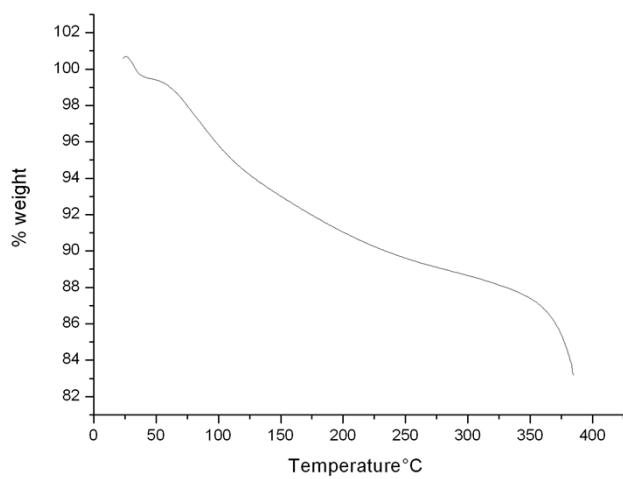
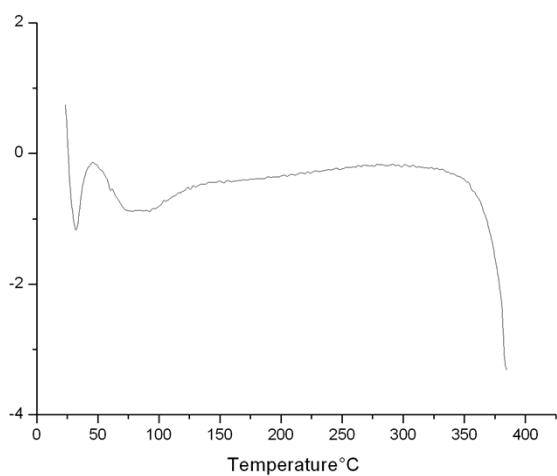
**Figure S4.**  $^1\text{H}$ -NMR spectrum of the photoreaction products of **1** (1 h of irradiation) in alkaline  $\text{D}_2\text{O}$  solution.



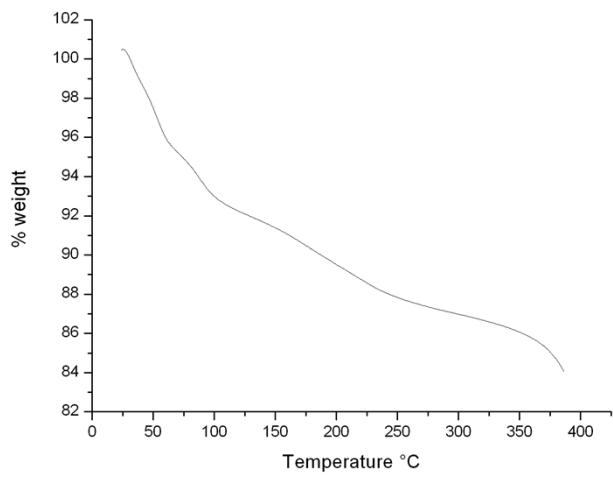
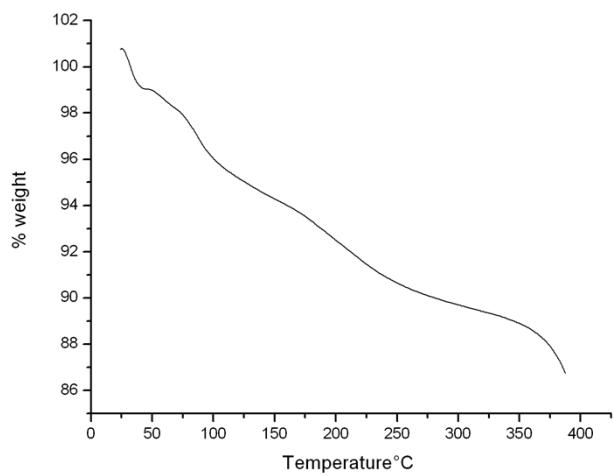
**Figure S5.(a)** Conformations of the hexadiendionc dianion and the photoproducts, in the anionic form, as obtained from DFT calculation.



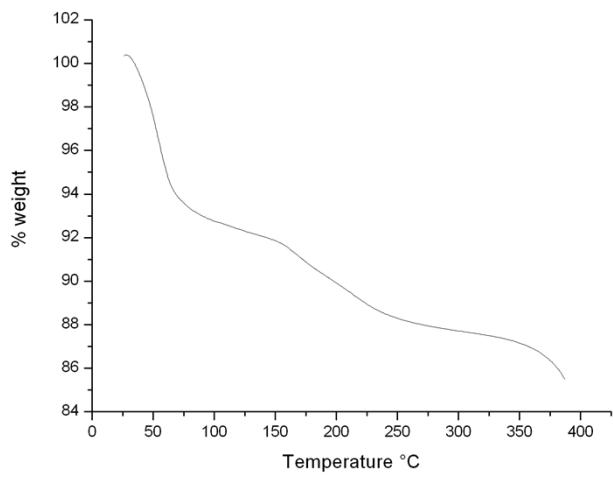
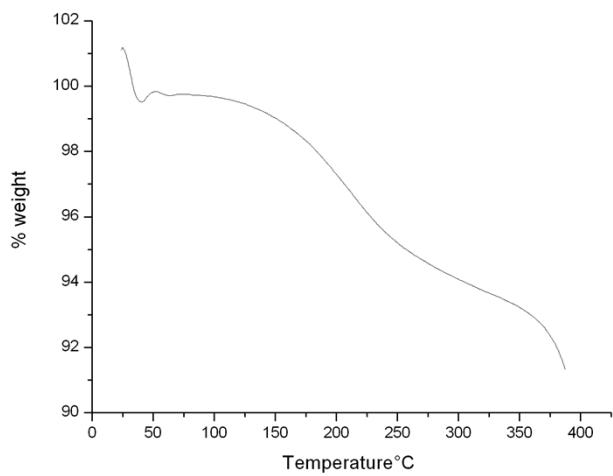
**Figure S5(b).** Calculated and experimental chemical shifts of the hexadienidion dianion and all photoproducts( in the anionic form).



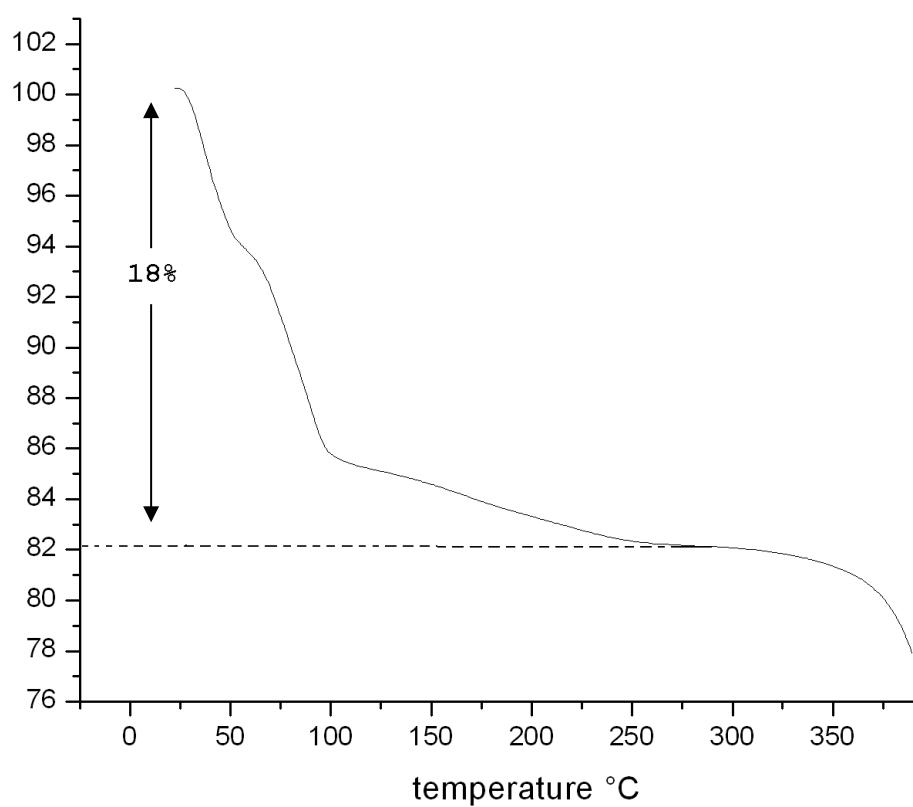
**Figure S6.** From bottom to the top: DSC analysis, TG analysis and DTG analysis of the photoproduct obtained after irradiation of compound **1** for 1 hour.



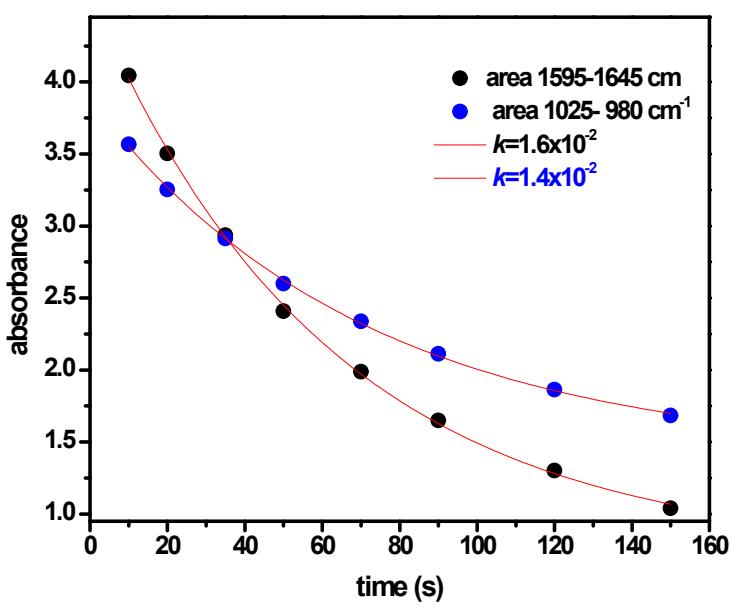
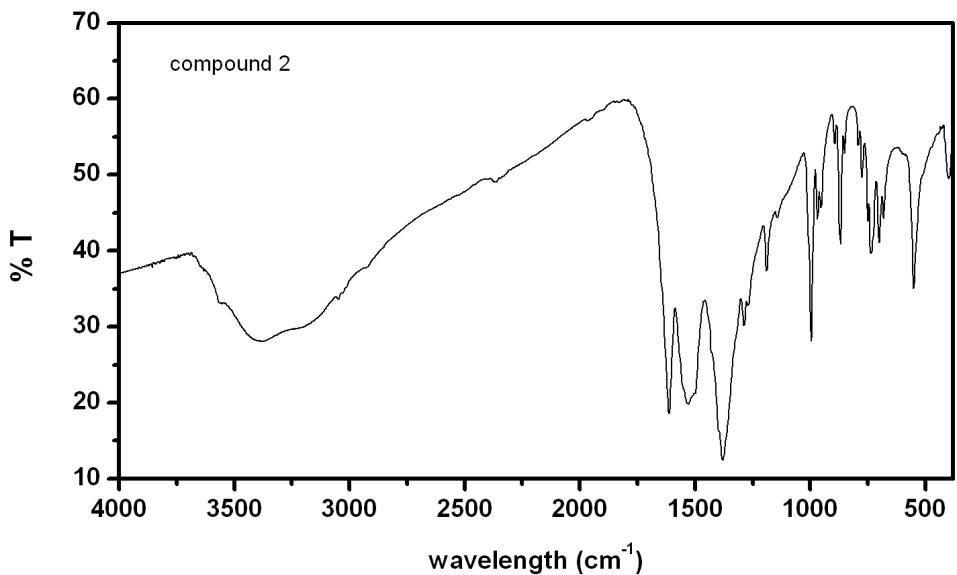
**Figure S7.(a)** TG analysis of hydrates **2** (top) and **2r** (bottom).



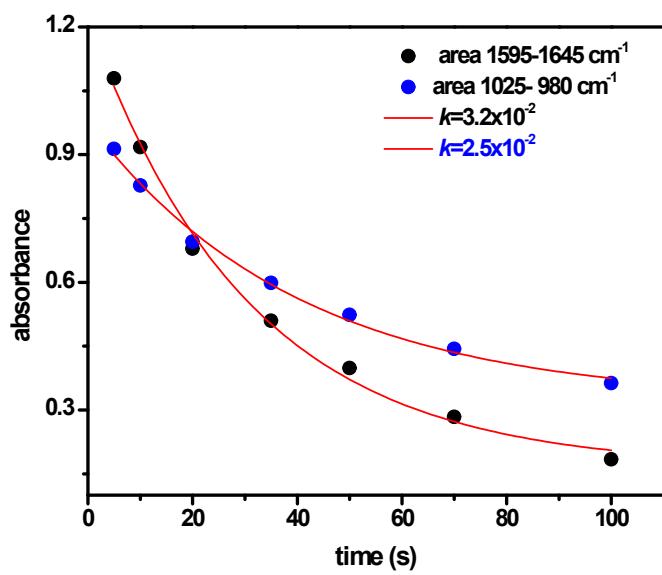
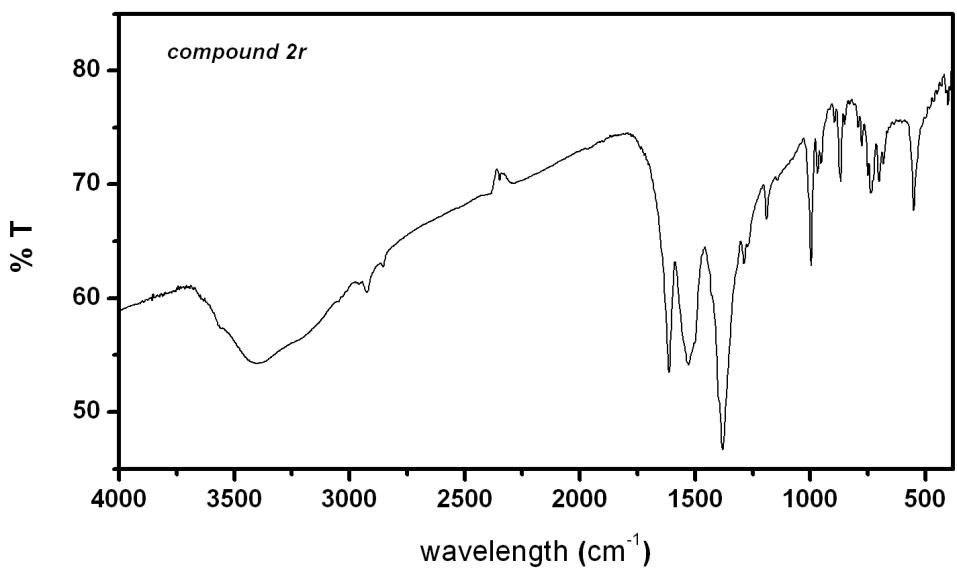
**Figure S7. (b)** TG analysis of hydrates **3** (top) and **3r** (bottom).



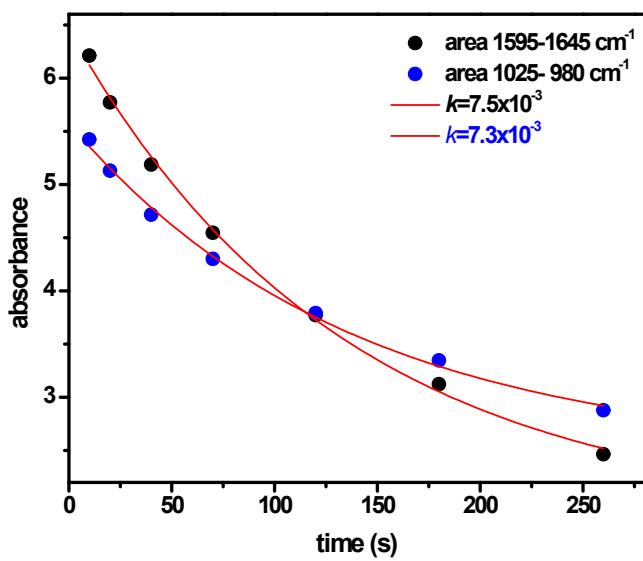
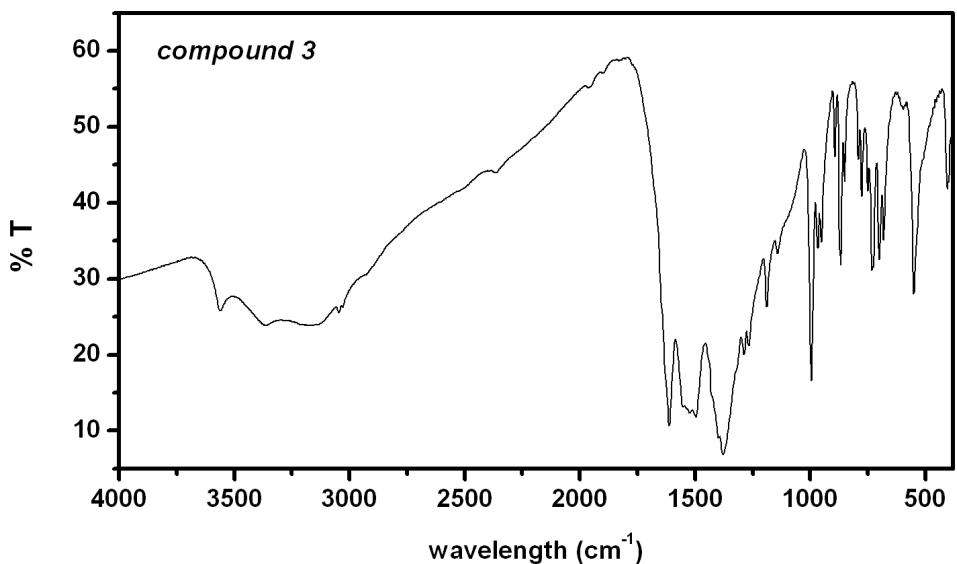
**Figure S7.(c)** TG analysis of hydrates 4.



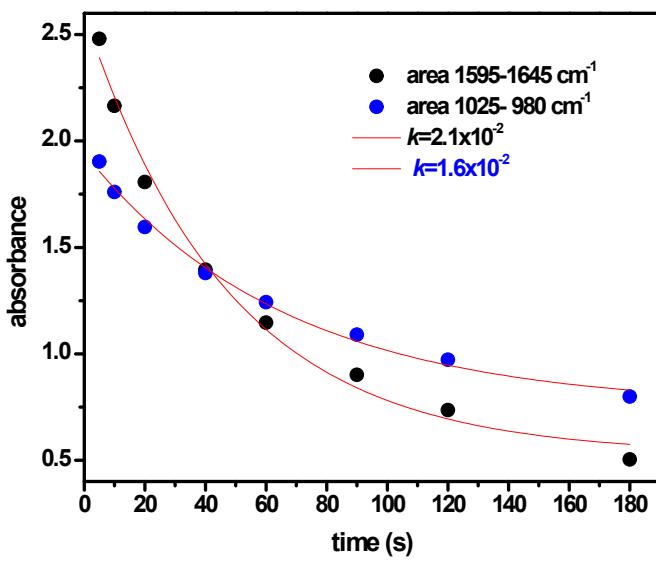
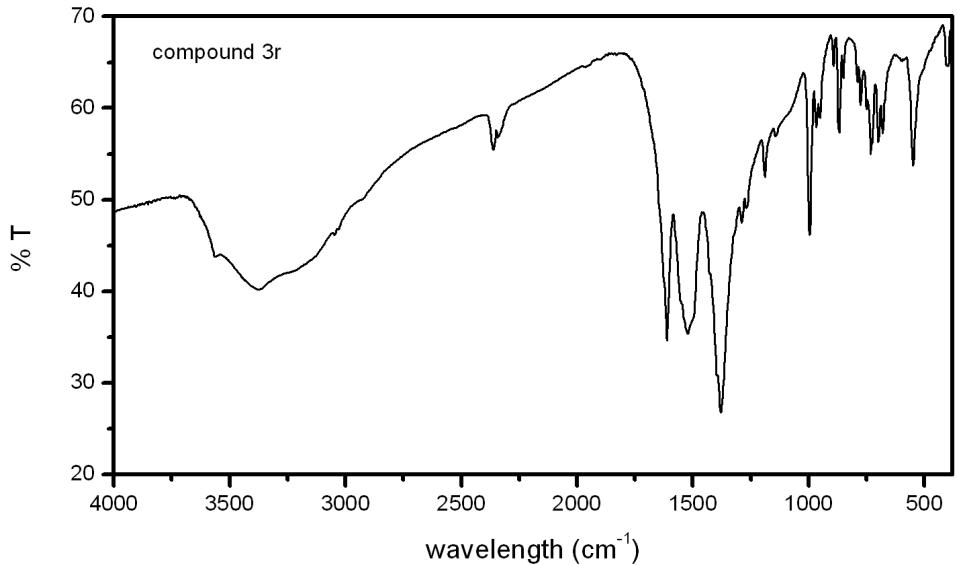
**Figure S8 (a).** Top: IR spectrum of compound 2. Bottom: Absorbance in two spectral regions as a function of irradiation time with the corresponding calculated reaction constants for compound 2.



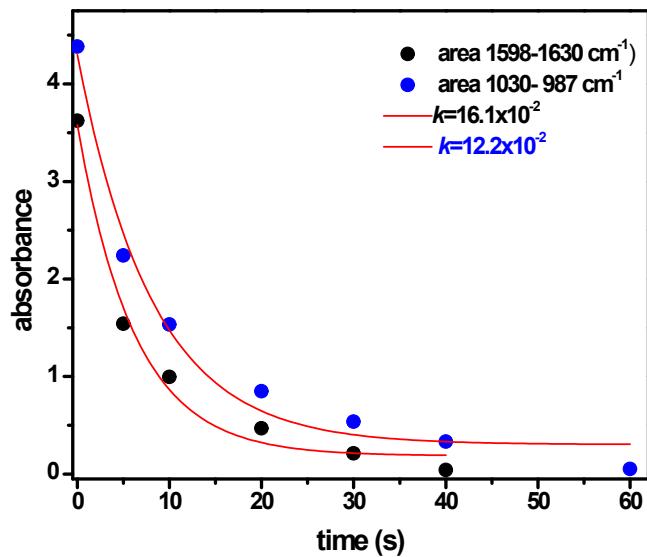
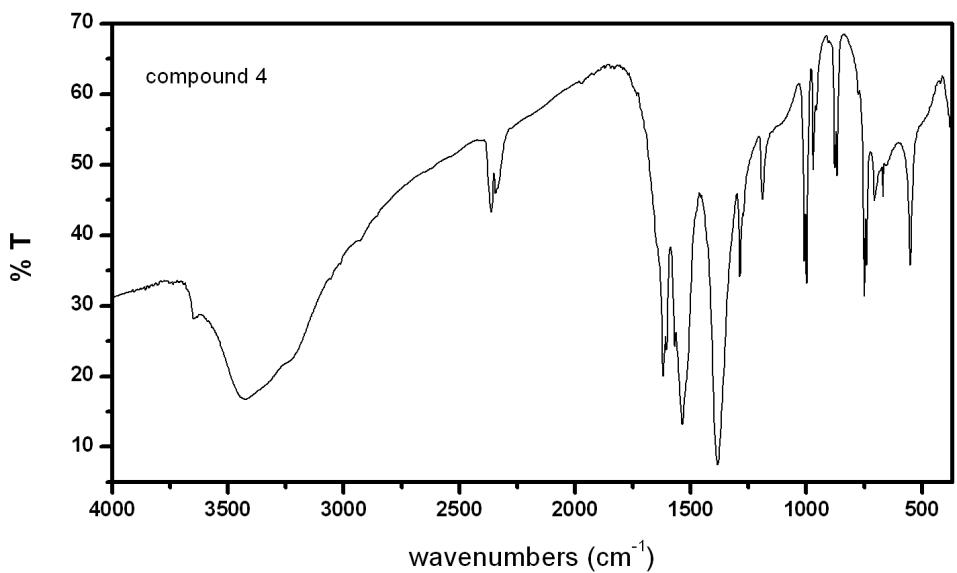
**Figure S8(b).** Top: IR spectrum of compound **2r**. Bottom: Absorbance in two spectral regions as a function of irradiation time with the corresponding calculated reaction constants for compound **2r**.



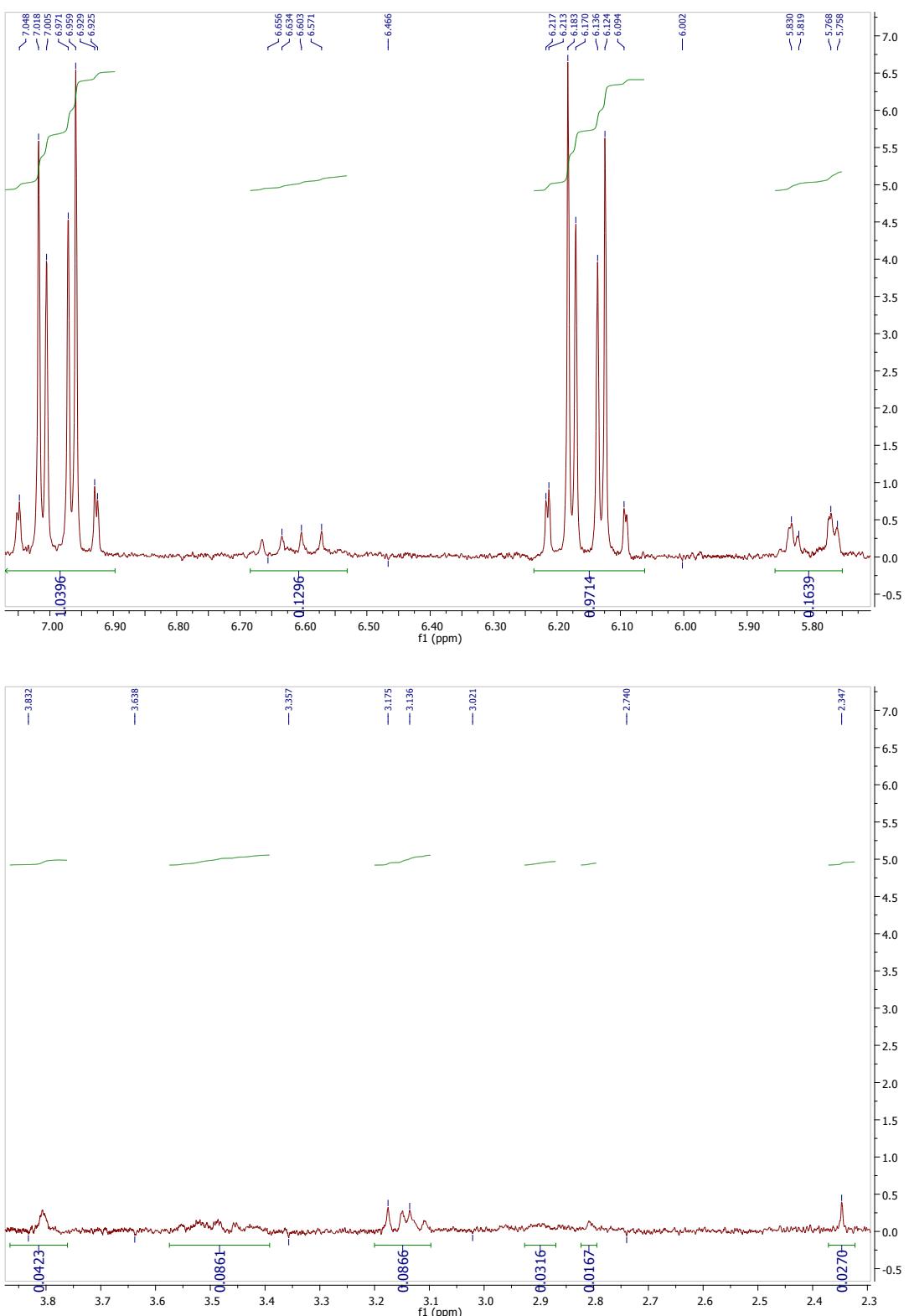
**Figure S8(c).** Top: IR spectrum of compound 3. Bottom: Absorbance in two spectral regions as a function of irradiation time with the corresponding calculated reaction constants for compound 3.



**Figure S8(d).** Top: IR spectrum of compound **3r**. Bottom: Absorbance in two spectral regions as a function of irradiation time with the corresponding calculated reaction constants for compound **3r**.



**Figure S8(e).** Top: IR spectrum of compound 4. Bottom: Absorbance in two spectral regions as a function of irradiation time with the corresponding calculated reaction constants for compound 4.



**Figure S9.**  $^1\text{H}$ -NMR spectrum of the photoreaction products of **3r** (6 h of irradiation) in alkaline  $\text{D}_2\text{O}$  solution.