Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

A 2D to 3D Solvent Mediated Transformation of a photoreactive lanthanum MOF: A case of three parallel photo-cycloaddition reactions

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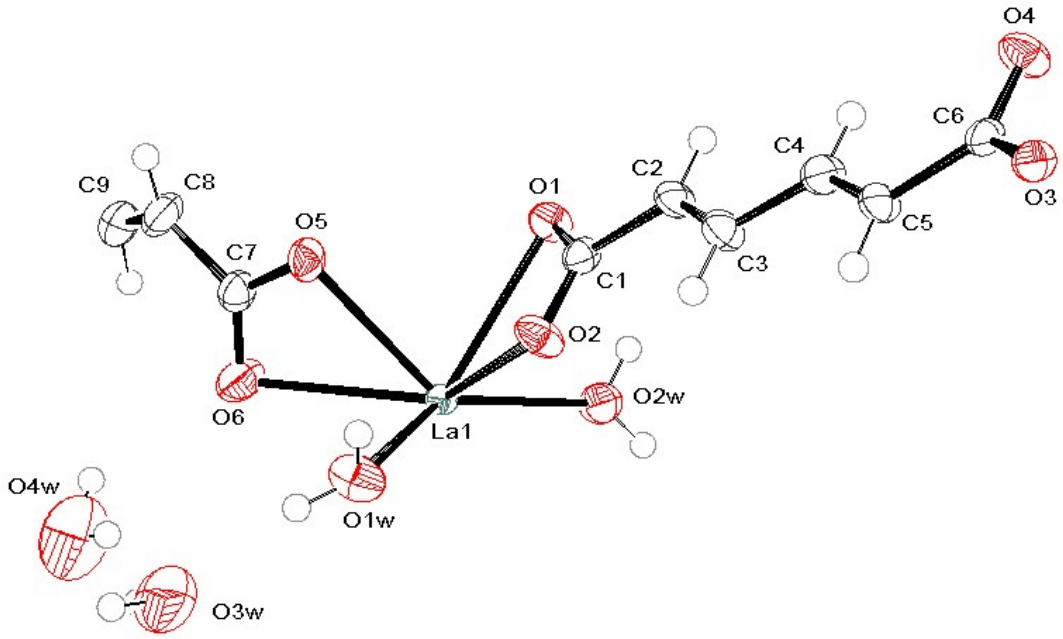

Fig. S1. ORTEP drawing of the asymmetric unit of compound 1.

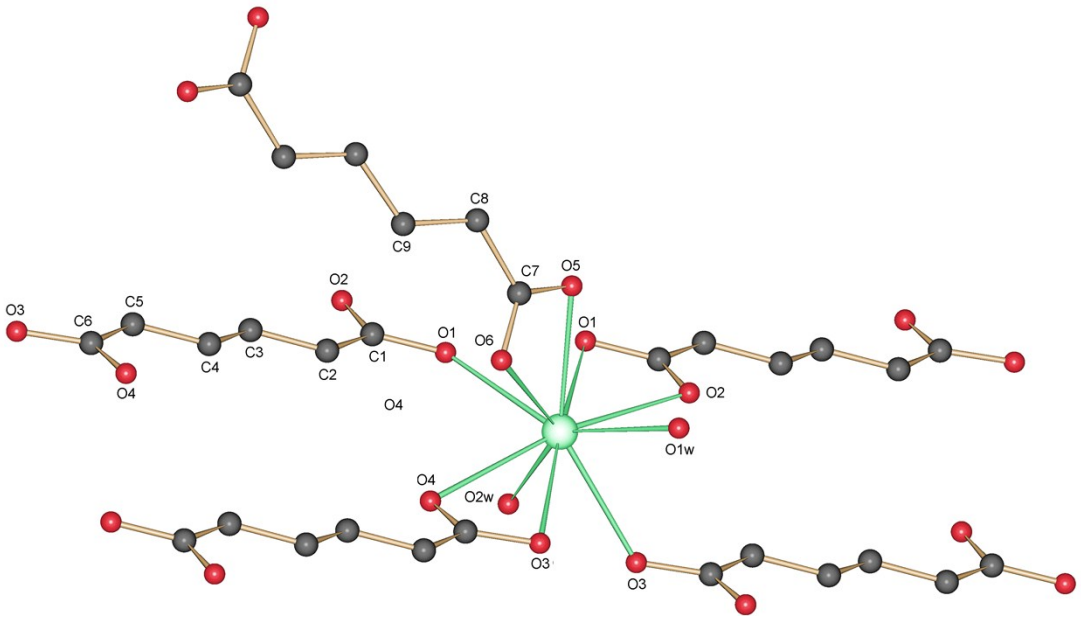

Fig. S2. Coordination environment of a lanthanum cation.

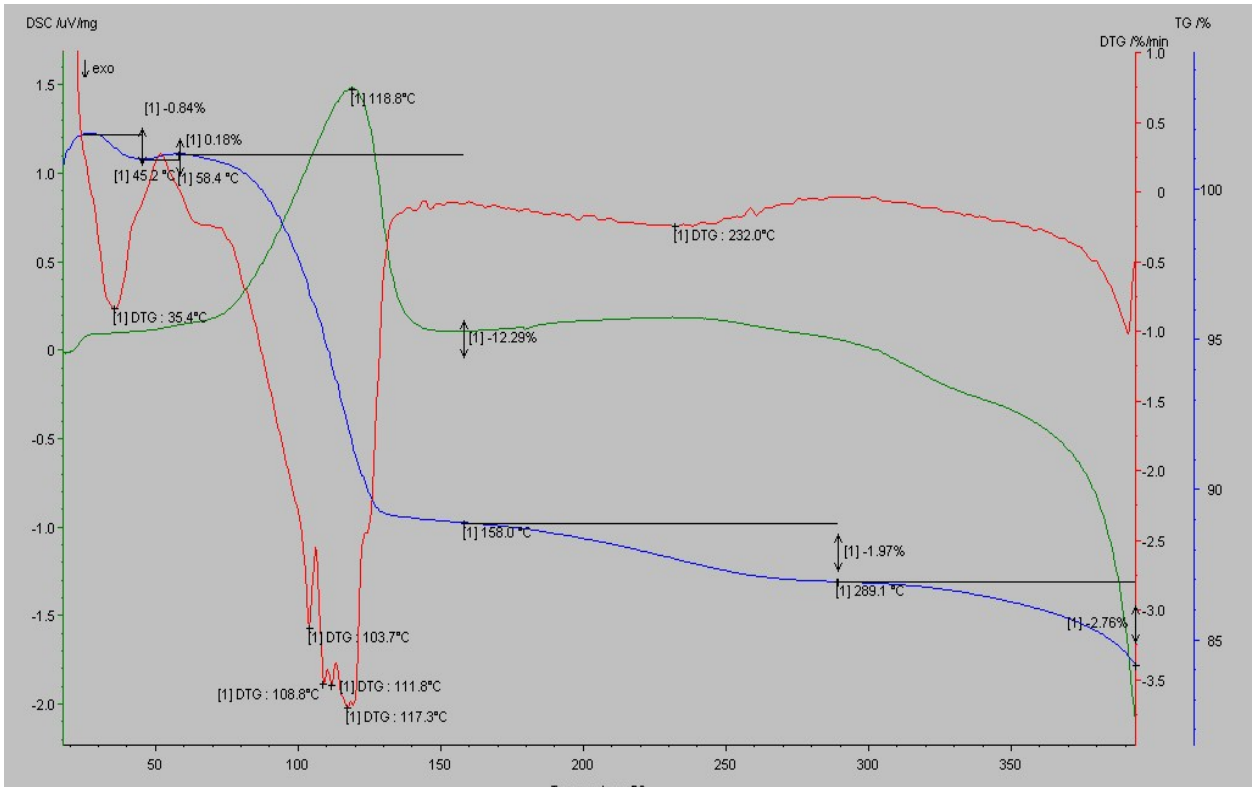

Fig. S3. TG/DTG/DSC diagram of compound 1.

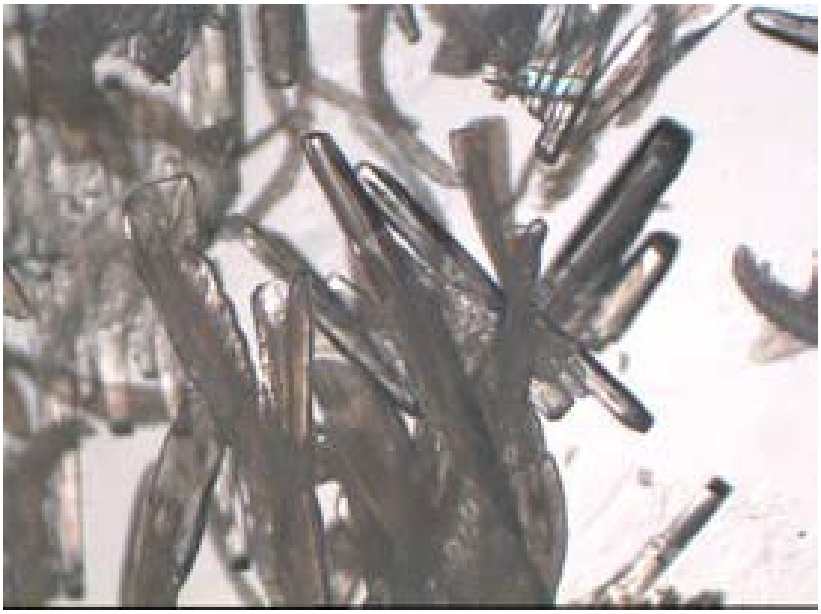

Fig. S4. Crystal morphology of compound 2.

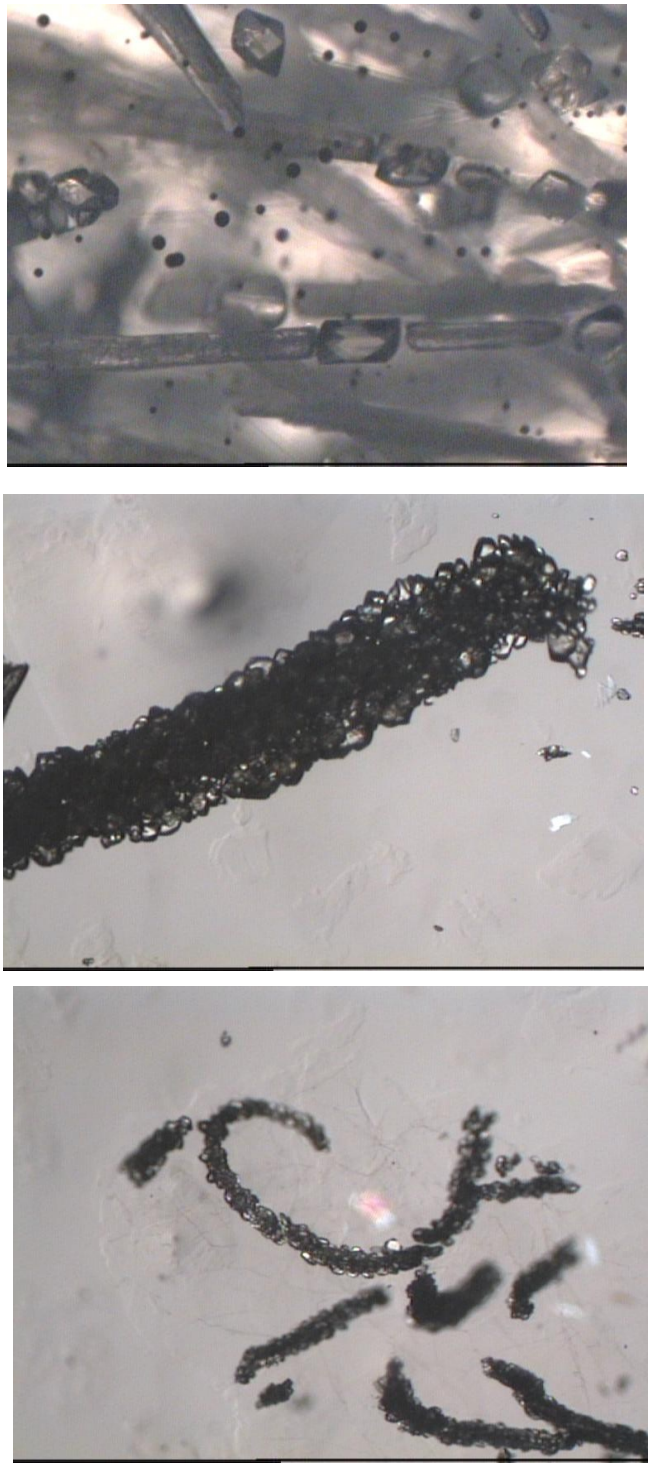

Fig. S5. Crystallization of compound 1 by in situ transformation of compound 2.

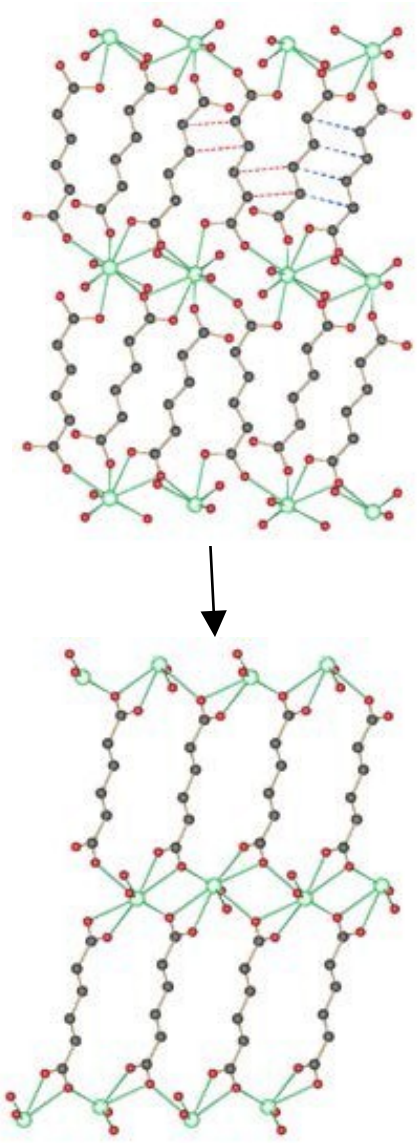

Fig. S6. Projection of the layer of the two MOFs. Cleavage of one metal-carboxylate bond in MOF 2 (top) takes place during transformation to MOF 1 (bottom).The red and blue dashed lines (top) connect olefinic carbons with a mean distance of 4.03 and and 3.80 Å respectively.

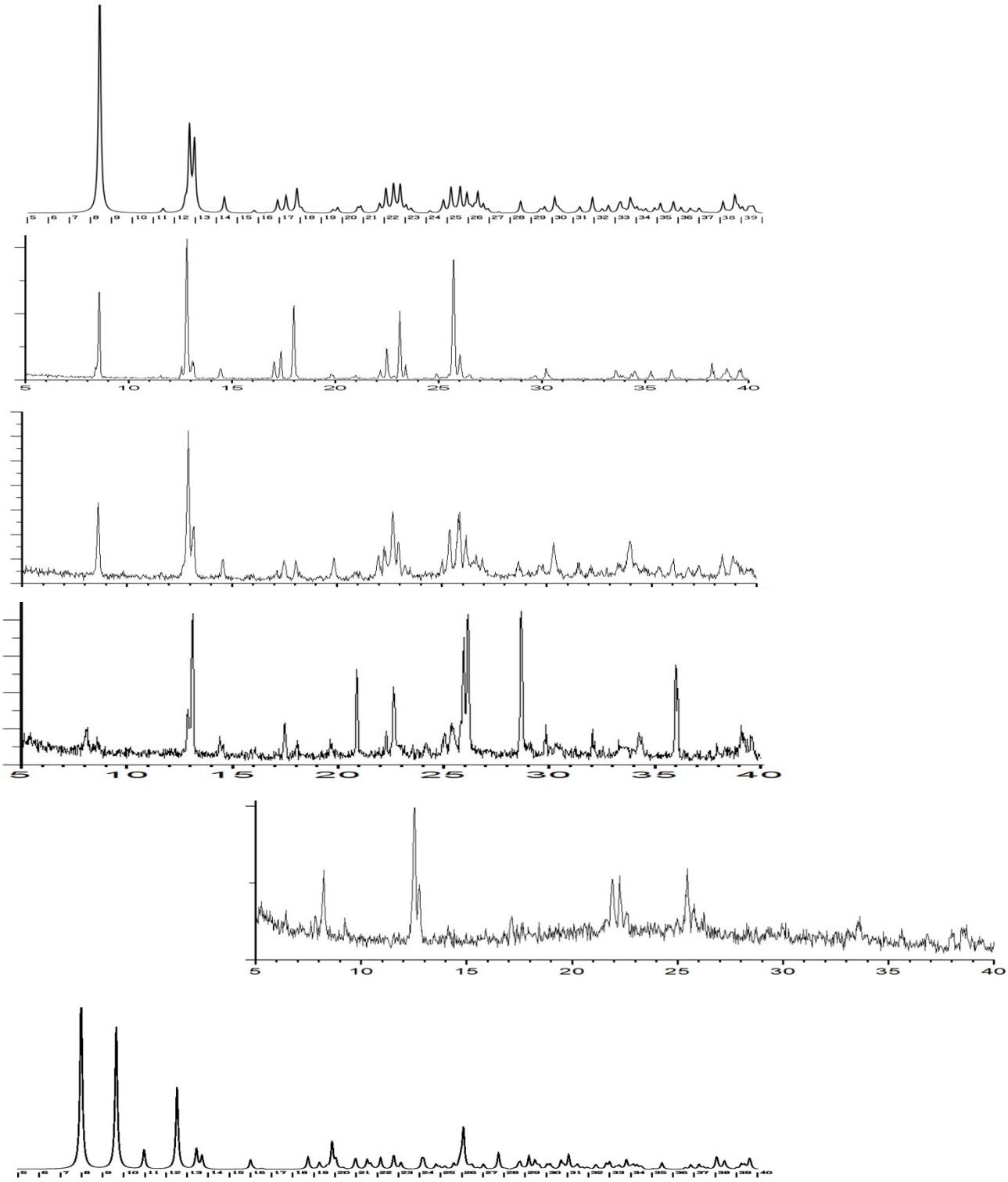

Fig. S7. From up to down: simulated PXRD pattern of 1, experimental PXRD pattern of 1, pattern of a powder of 2 in water heated at 50°C for six weeks, pattern of single crystals of 2 in water heated at 50°C for six weeks, pattern of a powder of 2 under an atmosphere of water vapor heated at 50°C for six weeks, simulated pattern of 2.

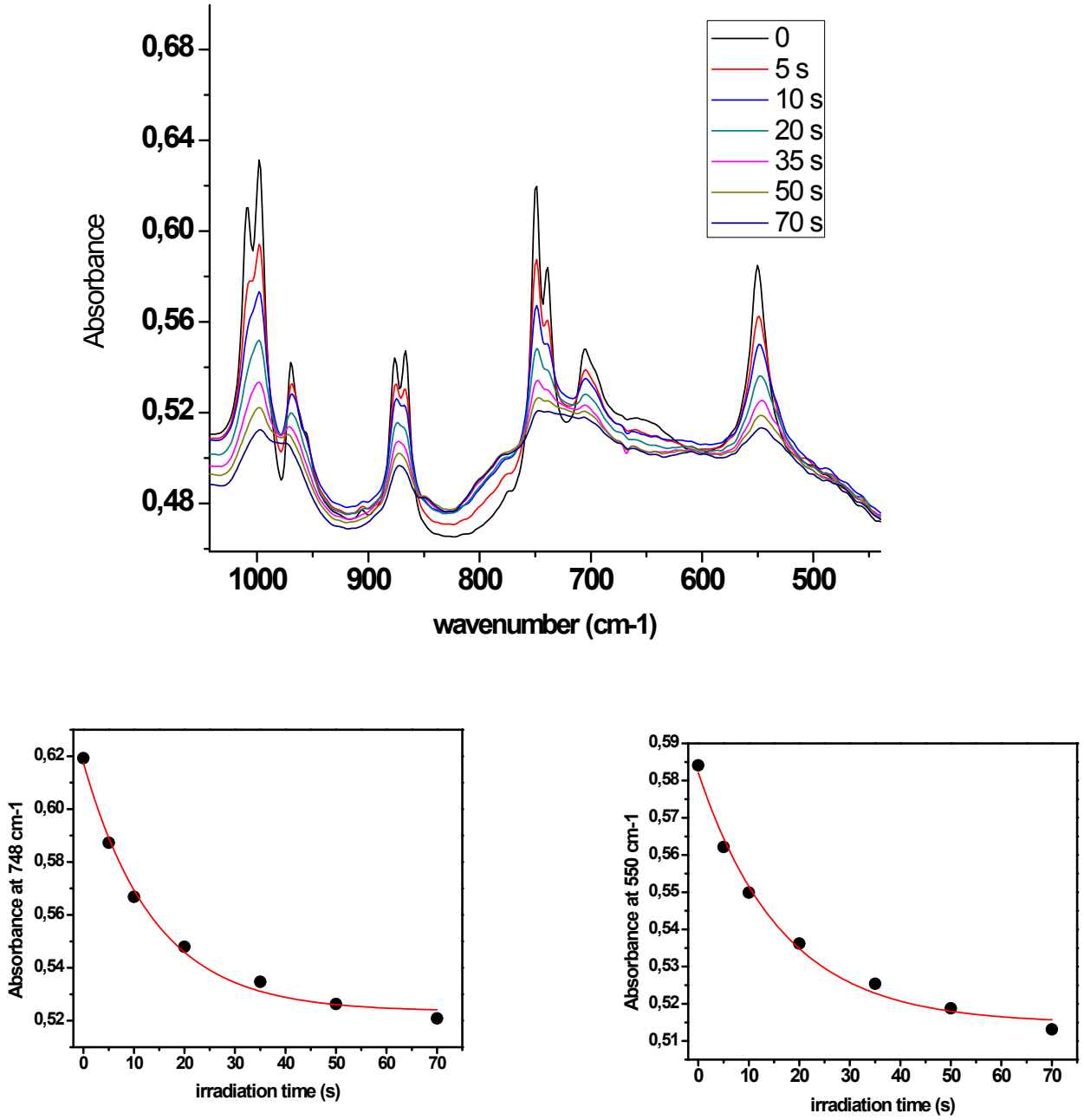

Fig. S8. (Top) IR spectrum of compound 1 obtained at different irradiation times. (Bottom) Absorbance in two spectral regions as a function of irradiation time.

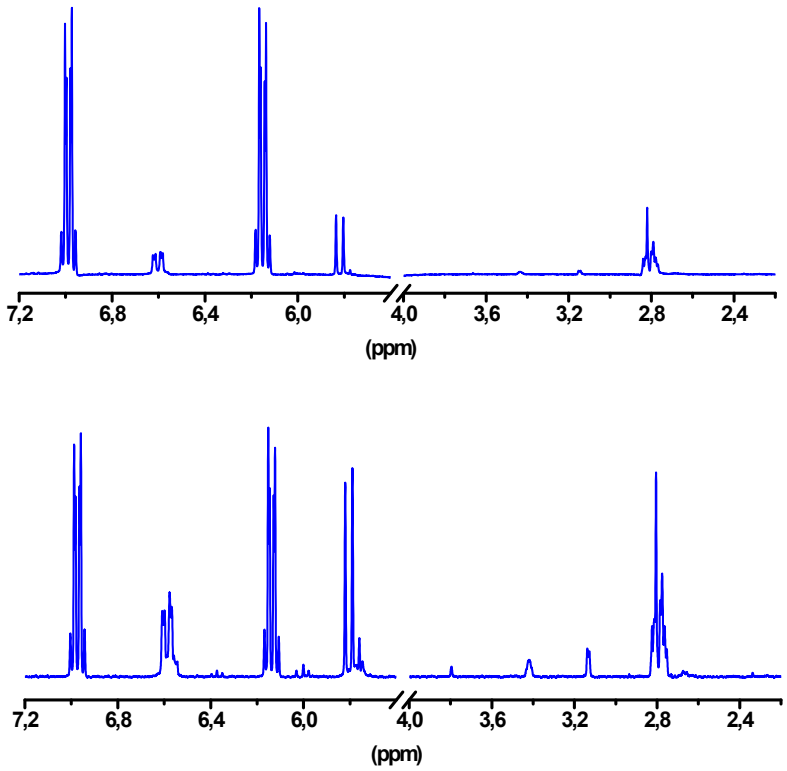

Fig. S9. ^{1}H-NMR spectra of compound 1 in D_2O alkaline solution, after 10 min of irradiation (top) and 30 min of irradiation (bottom).

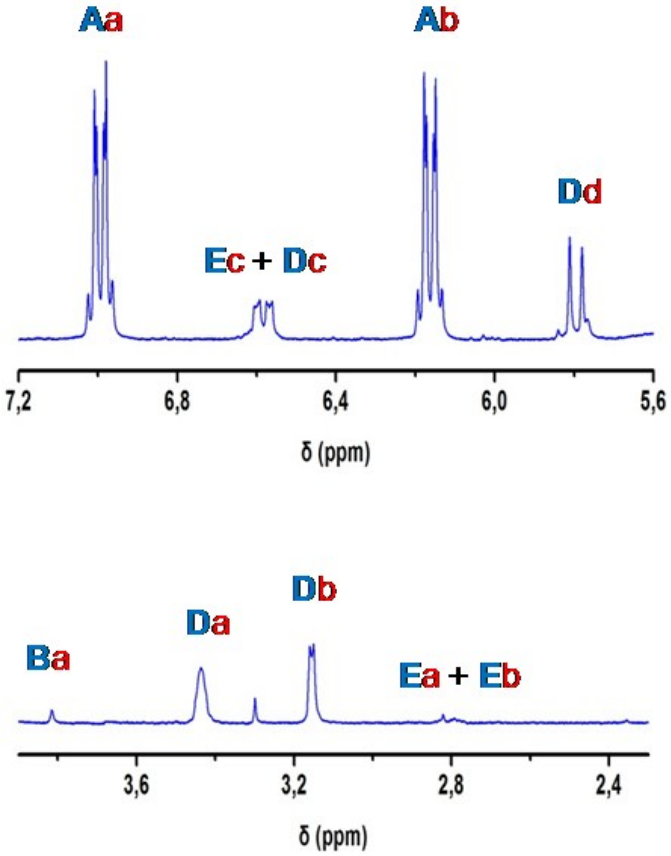

Fig. S10. ^{1}H-NMR spectrum of compound 2 in D_2O alkaline solution, after 1 h of irradiation. The proton symbols are as in Fig.5.

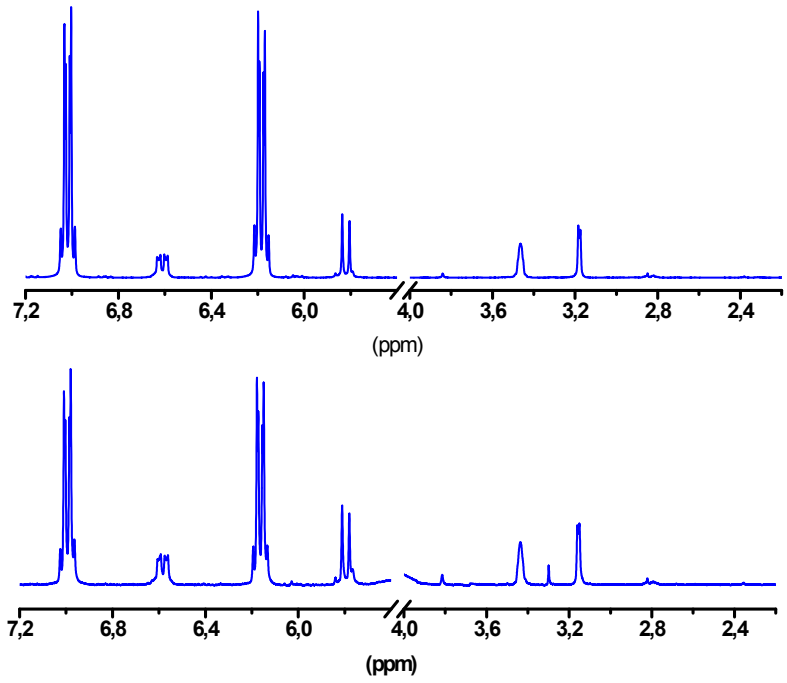

Fig. S11. ^{1}H-NMR spectra of compound 2 in D_2O alkaline solution, after 10 min of irradiation (top) and 30 min of irradiation (bottom).