Supplementary Information

Structural insight into the photoinduced $E \rightarrow Z$ isomerisation of cinnamate embedded in ZnAl and MgAl layered double hydroxides

Zita Timár[a,b], Gábor Varga[a,b], Márton Szabados[a,b], Krisztián Csankó[c], Tünde Alapi[d], Claude Forano[e], Vanessa Prevot[e], Pál Sipos[b,d], István Pálinkó[a,b*]

[a]*Department of Organic Chemistry, University of Szeged, Dóm tér 8, Szeged, H-6720, Hungary*
[b]*Materials and Solution Structure Research Group and Interdisciplinary Excellence Centre, Institute of Chemistry, University of Szeged, Aradi Vértanúk tere 1, Szeged, H-6720, Hungary*
[c]*Biological Research Centre, Temesvári krt. 62, Szeged, H-6726, Hungary*
[d]*Department of Inorganic and Analytical Chemistry, University of Szeged, Dóm tér 7, Szeged, H-6720, Hungary*
[e]*Université Clermont Auvergne, CNRS, SIGMA Clermont, ICCF, F-63000 Clermont-Ferrand, France*

To whom correspondence should be addressed.
E-mail: palinko@chem.u-szeged.hu (I. Pálinkó)

Table S1

The determined cell parameters and interlayer distances of the pristine LDH and the composites as well as the differences in asymmetric and symmetric vibrations of the carboxylate groups of the interlayered cinnamate isomers.

LDH composites	a (Å)	c (Å)	Interlayer distance (Å)	$\Delta(\nu_{as}(COO^-)$-$\nu_s(COO^-))$ (cm^{-1})
Mg_2Al-NO_3	3.0	31.5	8.7	
Mg_2Al-E-Cin	3.0	58.1	17.7	143
Mg_2Al-Z-Cin	3.0	68.7	21.3	187
Mg_2Al-E-Cin (slurry, after irradiation)	3.0	58.8	18.1	160
Zn_2Al-NO_3	3.06	26.58	8.86	
Zn_2Al-*E*-Cin	3.05	53.14	17.71	143
Zn_2Al-*Z*-Cin	3.04	62.63	20.88	162
Zn_2Al-*E*-Cin (slurry, after irradiation)	3.0	57.9	17.7	160

Table S2

FT-IR data of Na-E-Cin, Na-Z-Cin, Mg_2Al-E-Cin, Mg_2Al-Z-Cin, Mg_2Al-NO_3 LDHs; assignments are according to ref. [39].

		Infrared vibration band (cm^{-1})			
Na-E-Cin	Mg_2Al-E-Cin	Na-Z-Cin	Mg_2Al-Z-Cin	Mg_2Al-NO_3	Assignment by ref. [39]
		608		623	δ(OMg,AlO)
	635	623	631	706	δ(OMg,AlO)
690	686	690	683		α(CCC)
721	717	710			Φ(CCC)+γ(CH)ar
773	777	758	764		γ(CH)ar+γ(HCCO)+γ(OC OC)
		799	791	795	ν(Mg,AlO6)
				830	δ(Mg,AlOH)
849	850	856	856		βs(COO-)+β(CH)cinn
878	880		882	883	γ(CH)ar
		932	941		
972	978		968		γ(CCH)cinn
		1005	1007		α(CCC)+ ν(CCC)
		1032	1032		β(CH)ar+ ν(CC)ar
1074	1070	1074	1076		β(CH)ar+ ν(CC)ar
		1182	1184		β(CH)ar+ ν(CC)ar
		1211	1211		
1244	1248				β(CH)cinn
1294	1290			1356	β(CH)cinn+ ν(CC)
		1357	1363		νs(COO^-)
		1386	1388	1386	β(CH)ar+ β(CH)cinn
1413	1394				νs(COO^-)
1450		1450			β(CH)+ ν(CC)ar
1498	1499	1491	1493		β(CH)+ ν(CC)ar
1546	1537	1562	1550		νas(COO^-)
	1576	1595			ν(CC)ar+ β(CH)+ α(CCC)
1639	1637	1647	1637	1643	ν(C=C)cinn

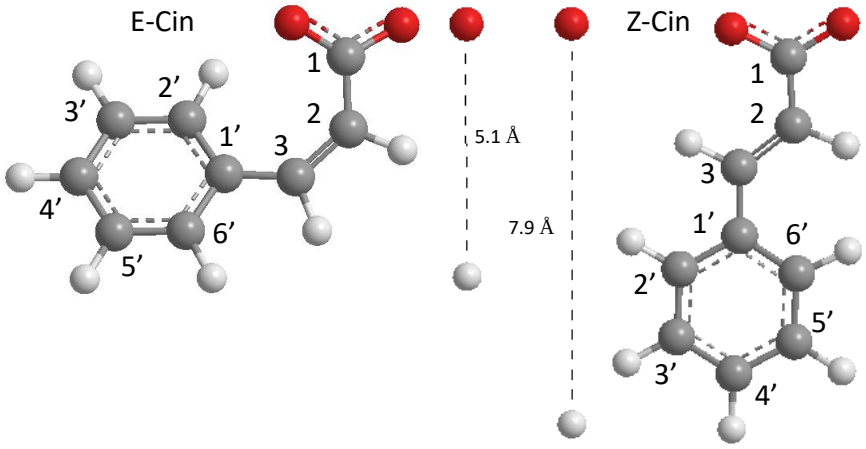

Fig. S1. Molecular structures of E-Cin and Z-Cin.

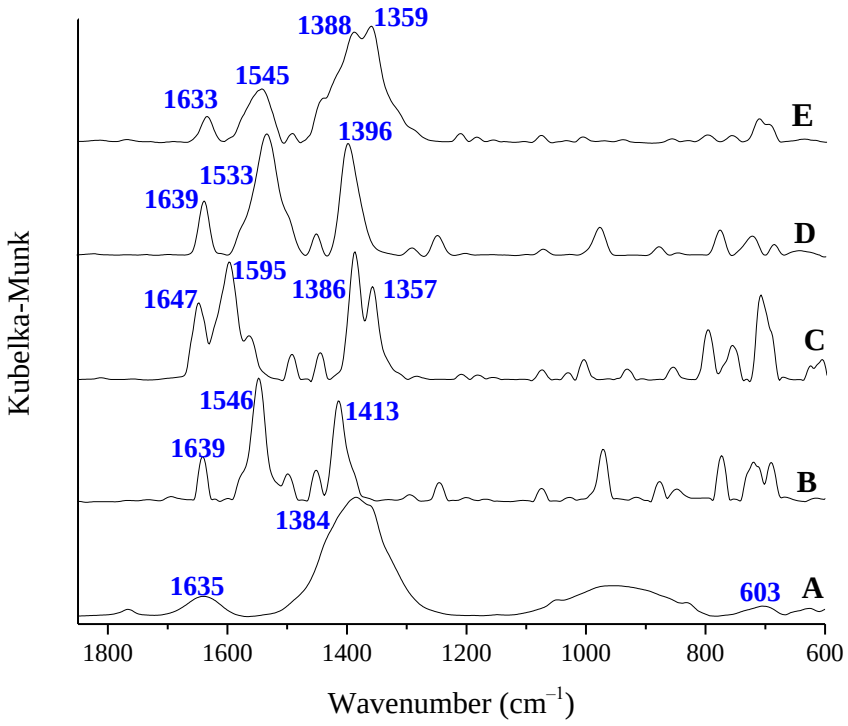

Fig. S2. IR spectra of the A: pristine Zn_2Al-LDH, B: sodium E-cinnamate, C: sodium Z-cinnamate, D: Zn_2Al-E-Cin LDH, E: Zn_2Al-Z-Cin LDH.

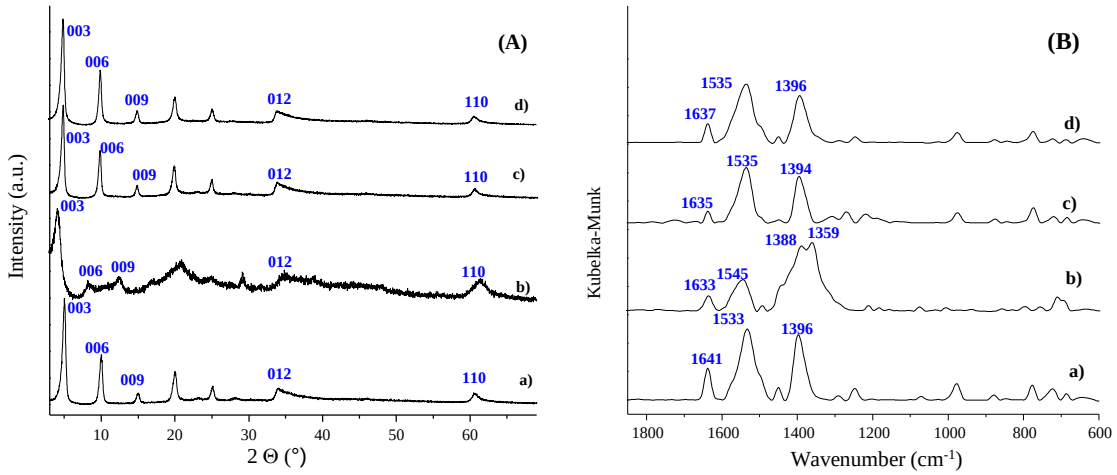

Fig. S3 (A) X-ray diffractograms and (B) IR spectra of a) Zn_2Al-E-Cin LDH, b) Zn_2Al-Z-Cin LDH, c) Zn_2Al-E-Cin LDH (solid state) irradiated at 254 nm for 2 h, d) Zn_2Al-E-Cin LDH (slurry phase – suspended in methanol) irradiated at 254 nm for 2 h.

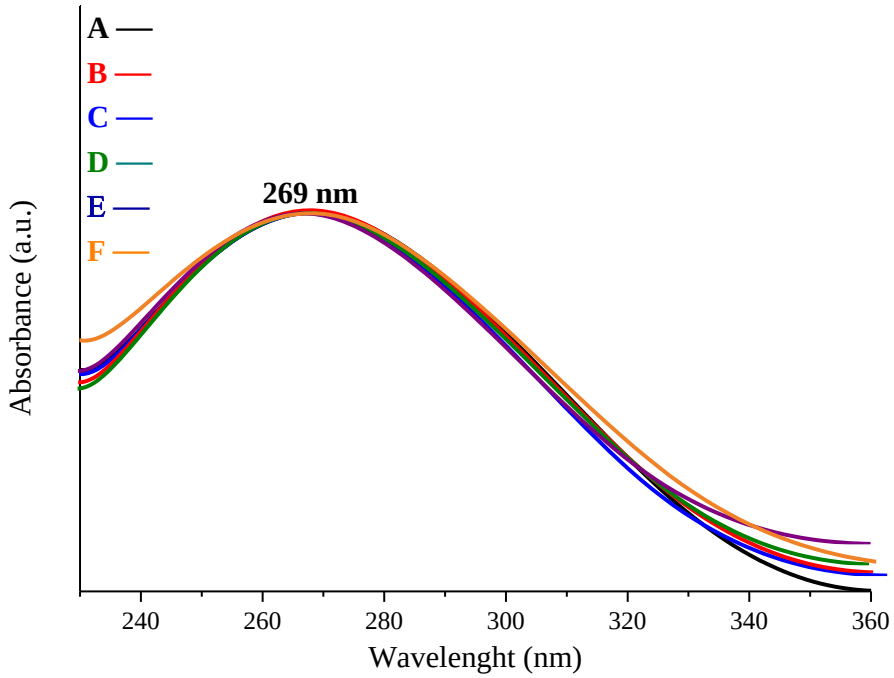

Fig. S4. UV-Vis spectra of the supernatants of the mixture of sodium E-cinnamate and Mg_2Al LDH, A: before irradiation, after various irradiation times, B: 1 h, C: 2 h, D: 3 h, E: 4 h and F: 24 h.

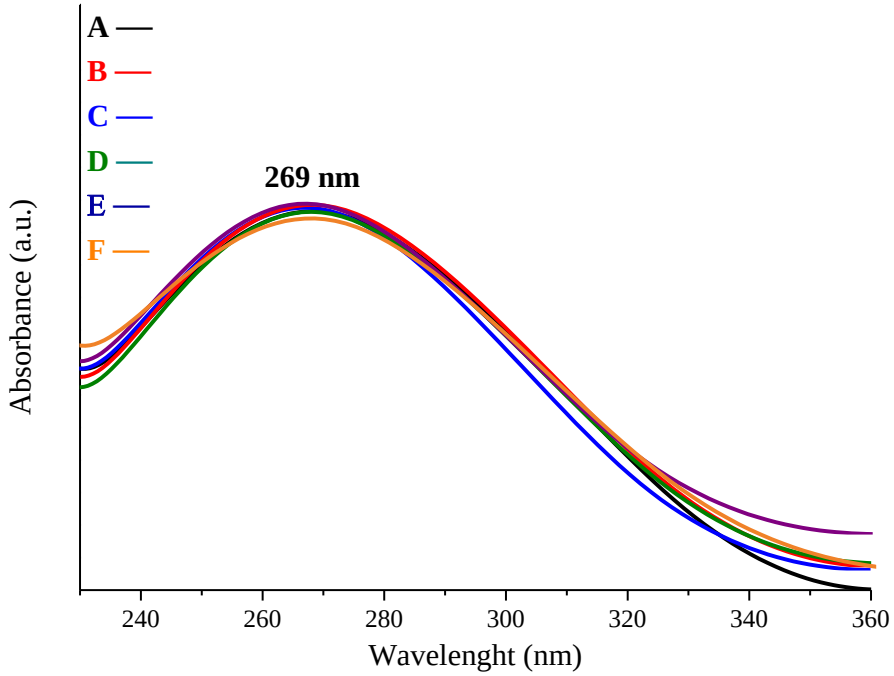

Fig. S5. UV-Vis spectra of the supernatants of the mixture of sodium *E*-cinnamate and Zn_2Al LDH A: before the irradiation, after various irradiation times B: 1 h, C: 2 h, D: 3 h, E: 4 h and F: 24 h.

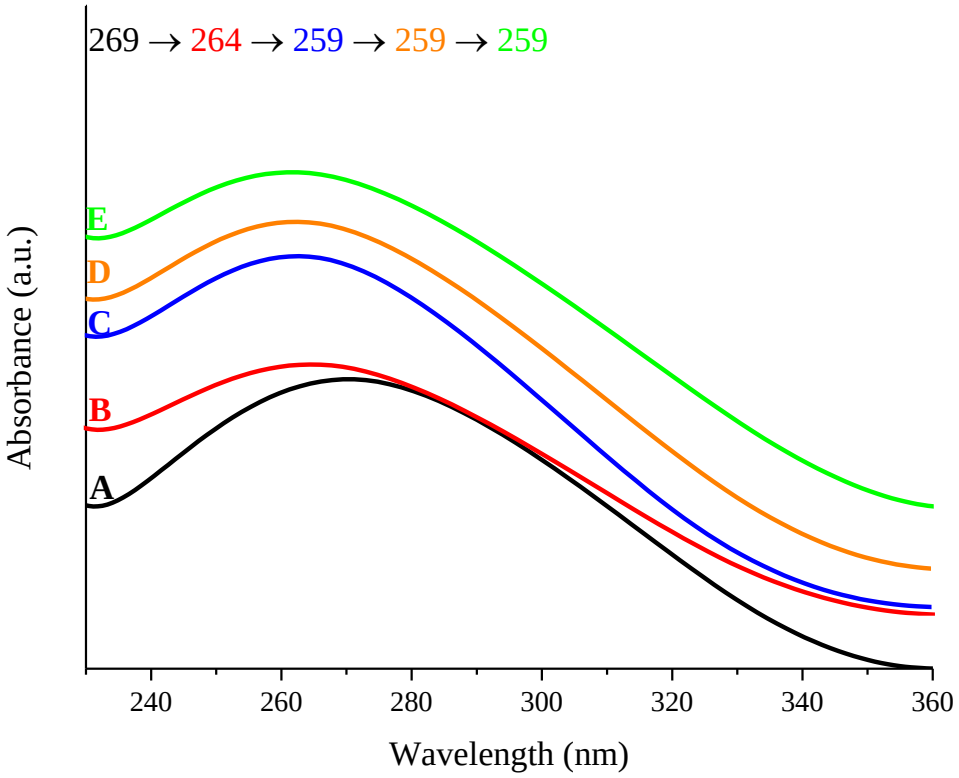

Fig. S6. UV-Vis spectra of the supernatants of ZnAl-E-Cin LDH A: before irradiation, after irradiation for B: 1 h, C: 2 h, D: 3 h and E: 4 h.