



Supplement of

LED-based solar simulator to study photochemistry over a wide temperature range in the large simulation chamber AIDA

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Table S1: Experimental conditions:

Photolysis of 2,3-pentanedione					
starting concentration [ppb]	illumination [min]	relative humidity [%]	temperature [K]		
66	65	12	213		
66	65	< 1	243		
20	65	1	273		
67	60	< 1	283		
71	60	< 1	298		
71	15 (intervals)	< 1	298		
Photolysis of DTDP					
DTDP	NH ₄ NO ₃ [mol l ⁻¹]	(NH ₄) ₂ SO ₄ [mol l ⁻¹]	illumination [min]	relative humidity [%]	temperature [K]
1 ml of prepared DTDP solution	0.026	-	120	75	283
1 ml of prepared DTDP solution	0.026	-	120	77	273
0.005 mol l ⁻¹	0.025	0.009	120	79	293
1 ml of prepared DTDP solution	0.026	-	120	70	264
Photosensitization experiments:					
Aerosol conc. [μg m ⁻³]	1 st illumination [min]	2 nd illumination [min]	relative humidity [%]	temperature [K]	
10 (solution 1)	67	64	87	283	
11 (solution 2)	60	61	72	243	
12 (solution 2)	60	60	55	213	
16 (reference solution)	61	-	88	283	
Solutions for photosensitization experiments					
	pinonic acid [mol l ⁻¹]	pinic acid [mol l ⁻¹]	NH ₄ NO ₃ [mol l ⁻¹]	Fe ₂ (C ₂ O ₄) ₃ (H ₂ O) ₆ [mol l ⁻¹]	oxalic acid [mol l ⁻¹]
solution 1	0.0065	0.0073	0.013	0.0021	-

solution 2	0.0064	0.0019	0.013	0.0021	-
reference solution	0.012	-	0.026	-	0.0081

Table S2: List of LEDs:

peak wavelength	LED model	producer	optical power [W]	number
305 nm	LEUVA77N50KU00 4in1	LG Innotek	0.3	6
	EOLS-310-637	EPIGAP	0.06	108
325 nm	EOLS-325-697	EPIGAP	0.56	802
340 nm	EOLS-340-697	EPIGAP	0.06	802
365 nm	LEUVA77Z80TV00 4in1	LG Innotek	5.0	32
	CUN66B1G	Seoul Viosys	1.8	50
385 nm	LEUVA77Z80TV00 4in1	LG Innotek	6.0	40
	CUN86B1G	Seoul Viosys	2.0	60
405 nm	LEUVA77Z80VV00 4in1	LG Innotek	6.0	40
	CUN06B1G	Seoul Viosys	2.0	80
415 nm	LEUVA33W70WL00	LG Innotek	1.9	27
420 nm	CUN26B1B	Seoul Viosys	1.04	54
455 nm	OSLON SSL GD CS8PM1.14	Osram	1.5	160
465 nm	OSLON SSL GB CS8PM1.13	Osram	1.06	224
528 nm	OSLON SSL GT CS8PM1.13	Osram	0.37	528

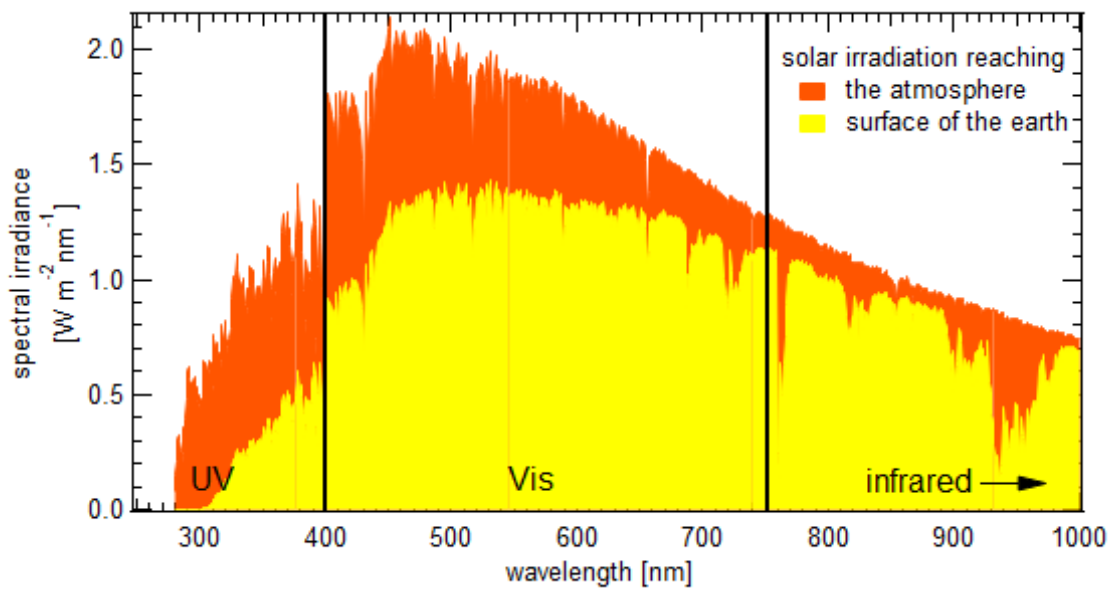


Figure S1: Solar Spectrum in the atmopshere derived from SMARTS v. 2.9.2 (ASTM G173-03 Reference Spectrum):

Reference: Data from United States Department of Energy, National Renewable Energy Laboratory, Reference Solar Spectral

10 Irradiance: ASTM G-173, <https://www.nrel.gov/grid/solar-resource/assets/data/astmg173.xls>

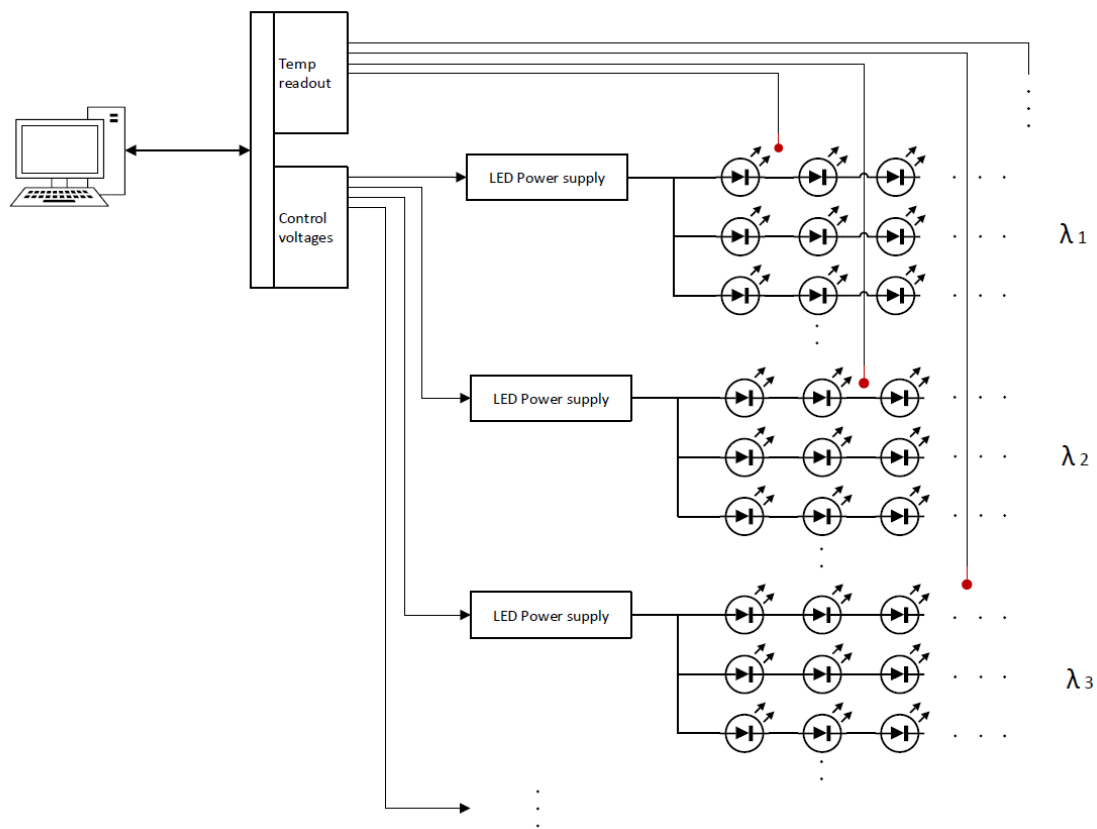
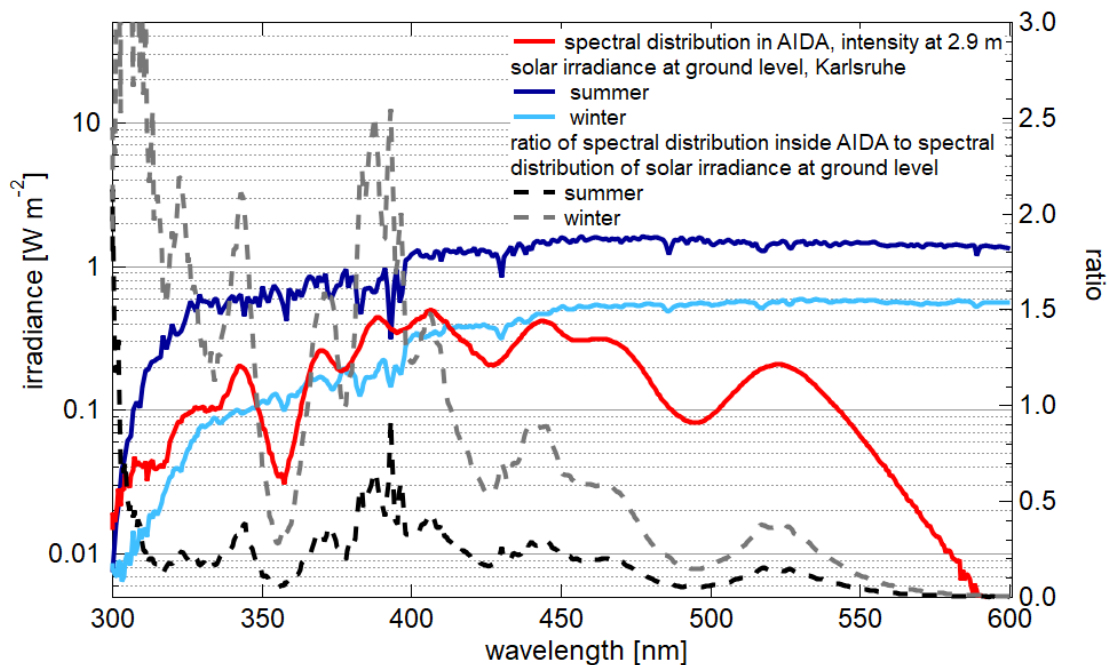
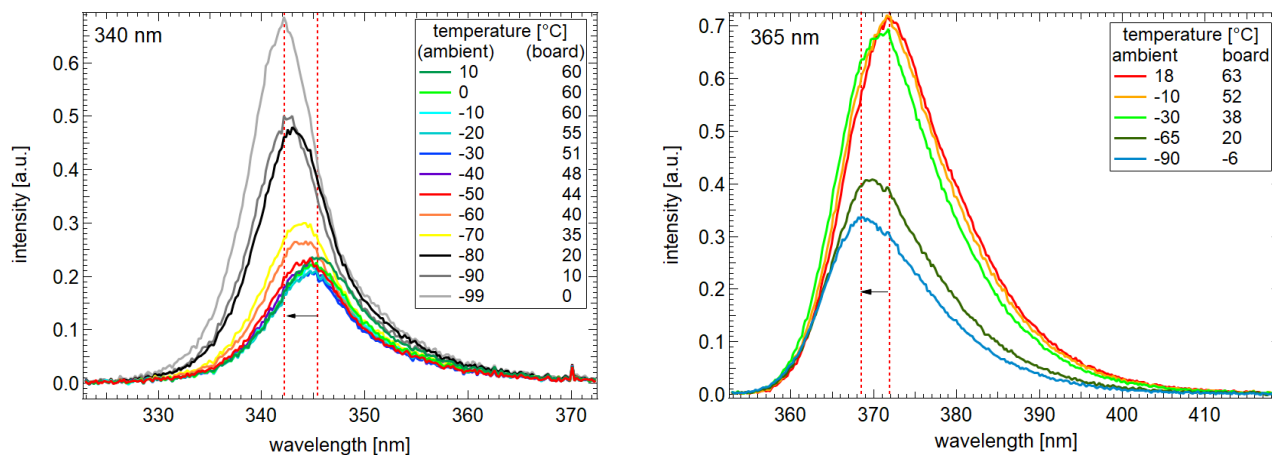


Figure S2: Electronic connection scheme for the LED power control and temperature readout.



15 Figure S3: Left axis: Spectra in summer and winter in Karlsruhe at ground level as well as in AIDA at 2.9 m. Right axis: Ratio of spectral distribution divided through the respective solar spectra.



20 Figure S4: Emission spectra of two LEDs at different ambient temperatures. The temperature of the LED-board can be different in the actual setting of the light source as the LED tests were made on a different heat sink.

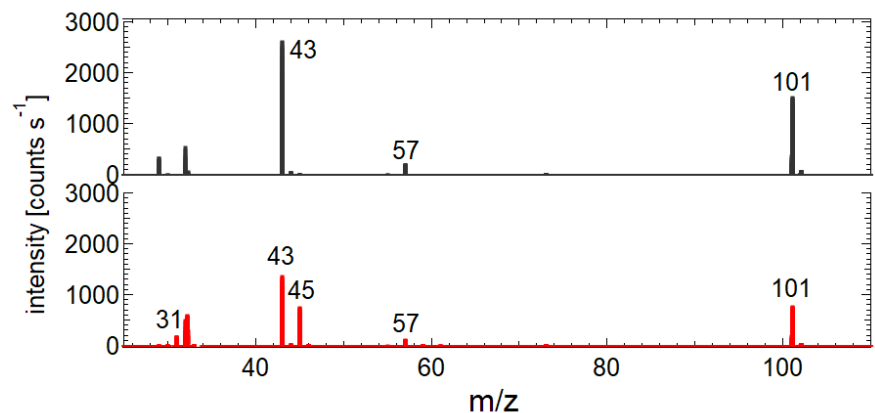


Figure S5: Mass Spectrum of 2,3-pentanedione before and after illumination (PTRMS): The mass peak for 2,3-pentanedione can be found at m/z 101. M/z 43 and m/z 57 refer to fragments of 2,3-pentanedione. M/z 45 and m/z 31 refer to the reaction products acetaldehyde and formaldehyde.

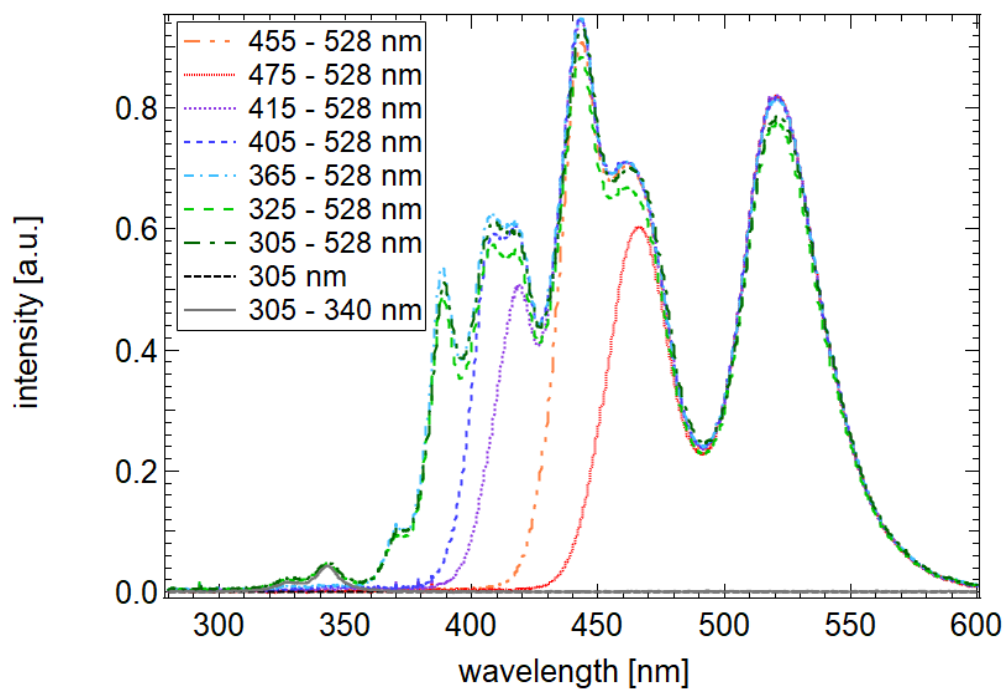


Figure S6: Spectra taken at the bottom of the chamber with different settings for the LEDs, resulting in different emission spectra of the light source.

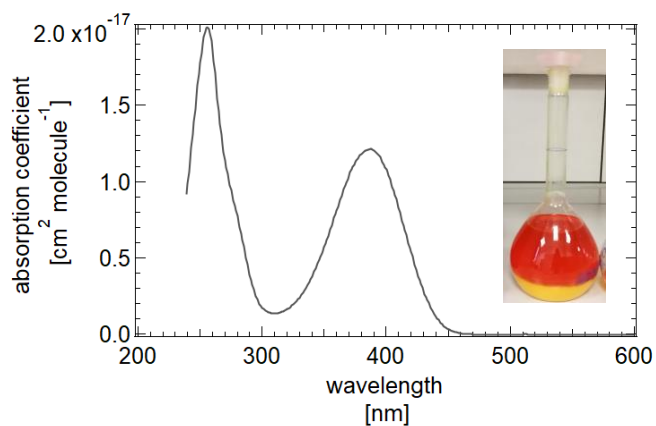


Figure S7: Absorption spectrum of 3,5-diacetyl-2,4,6-trimethyl-1,4-dihydropyridin ($19.25 \mu\text{mol l}^{-1}$ in water). Insert shows the red colour of the compound in a mixture of water and methanol after synthesis from acetaldehyde and 2,3-pentadione in presence of $(\text{NH}_4)_2\text{SO}_4$.

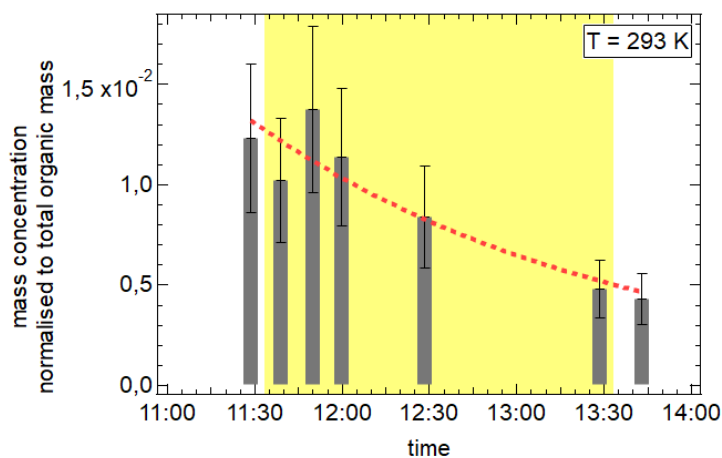


Figure S8: Mass concentration of 3,5-diacetyl-2,4,6-trimethyl-1,4-dihydropyridine in the particle phase at 293 K, normalised to the total organic mass of every filter measurement. The concentration decreases over the illumination period.

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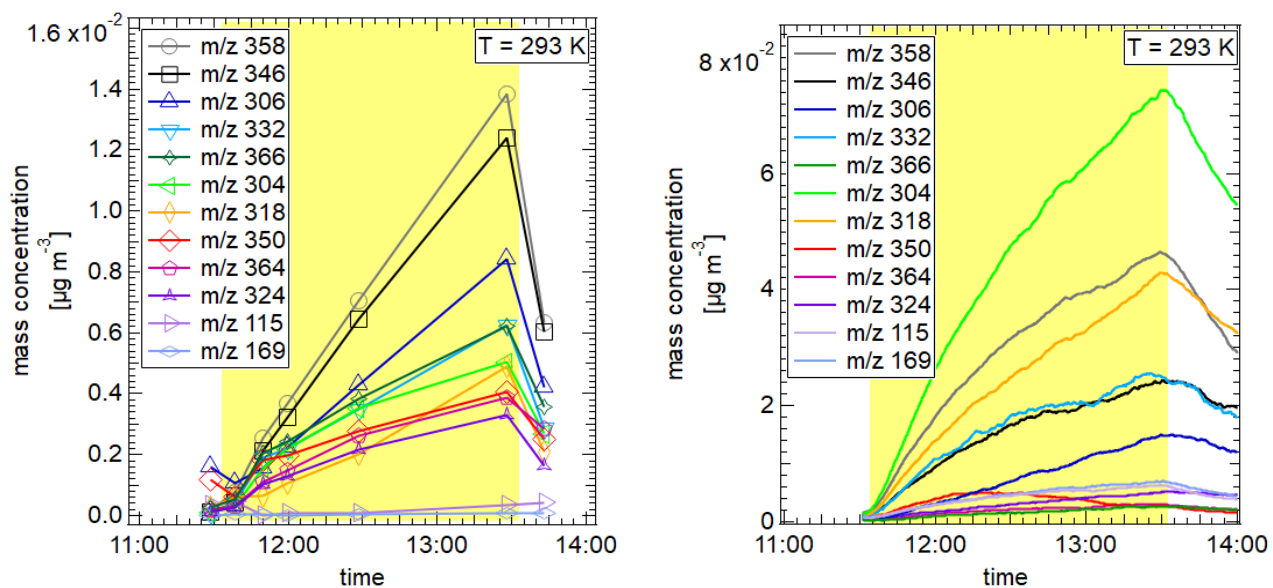
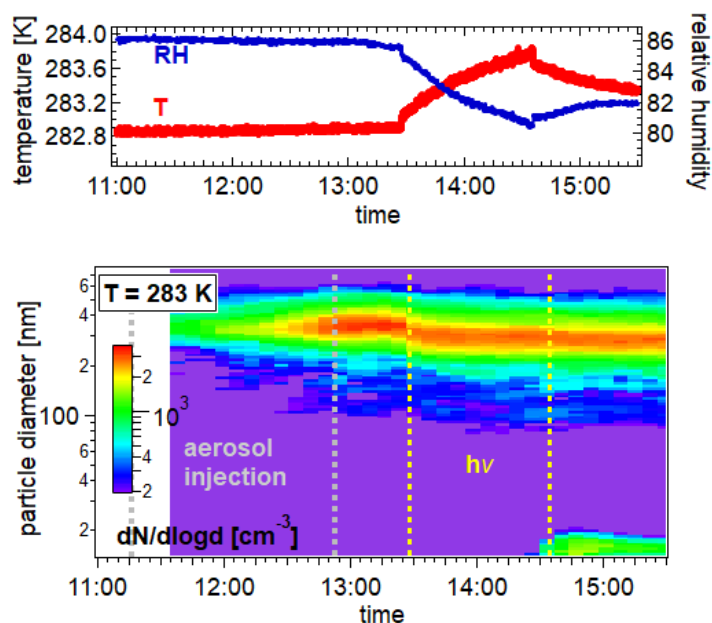


Figure S9: Mass increase of 16 components in particle (left) and gas phase (right) during illumination of an aerosol containing 3,5-diacetyl-2,4,6-trimethyl-1,4-dihydropyridine, $(\text{NH}_4)_2\text{SO}_4$ and NH_4NO_3 . The masses include the iodide used in the ionization process.



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Figure S10: temperature, relative humidity and particle size distribution over the course of one experiment. Aerosol injection and illumination period is marked separately. During illumination the temperature increases by 0.8 K. The sudden rise and

decrease of the temperature at the beginning and end of the illumination is due to the direct illumination of the temperature sensors. With increase of temperature, the relative humidity reduces by 5 percentage points. at the same time the particle diameter reduces by 50 nm.

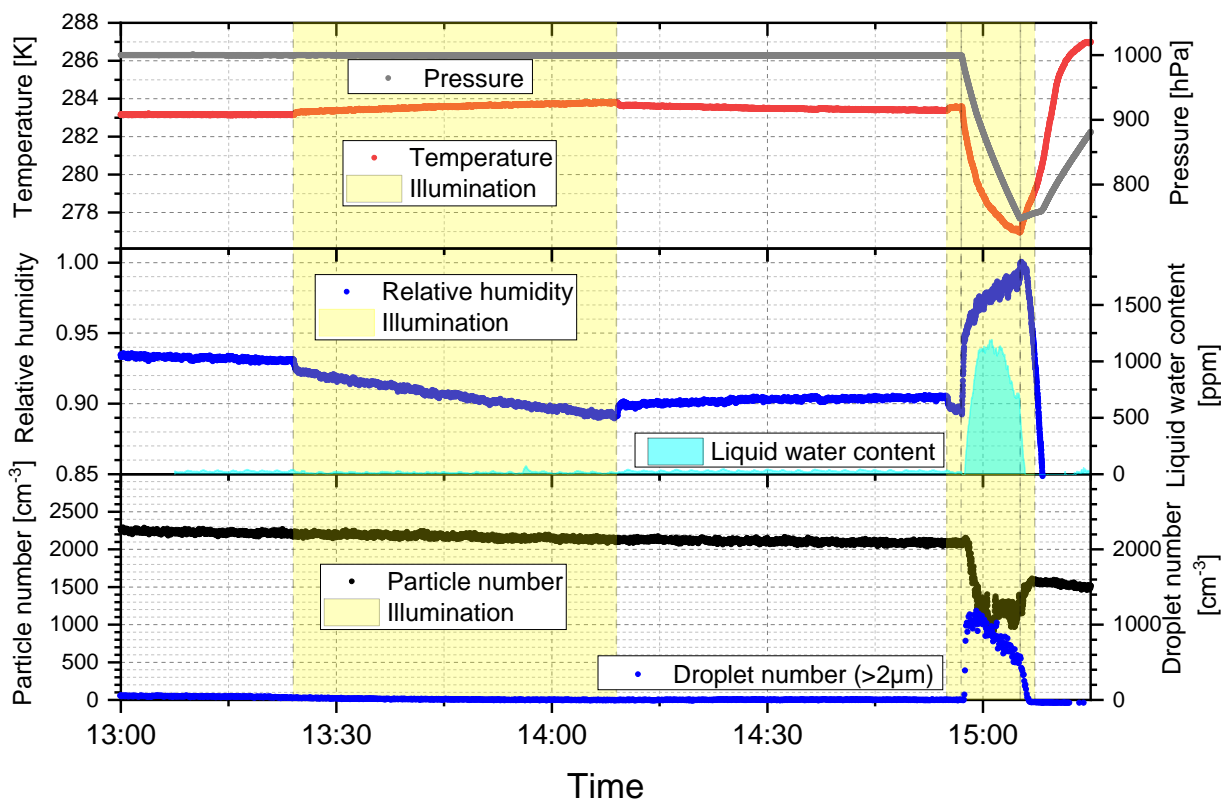


Figure S11: Aerosol particles of 60 wt.% NaCl + 20 wt.% humic acid + 20 wt.% nonanoic acid at 283 K and an initial relative humidity of 93 %. During the first illumination, the temperature increases and the relative humidity decreases correspondingly. During the second illumination an adiabatic expansion lead to an increase of the relative humidity resulting in an activation of about half of the aerosol particles as cloud droplets with a mean diameter of about $7 \pm 1 \mu\text{m}$. Please note that the stepwise change in temperature and relative humidity for switching on and off the light source is due to direct impact of radiation on the temperature sensors and not to a real sudden change in temperature.

Text S1: NO_2 -photolysis frequencies for the illumination conditions in Karlsruhe were calculated with the Quick TUV calculator of the National Center for Atmospheric Research (https://www.acom.ucar.edu/Models/TUV/Interactive_TUV/) for two days with the following settings:

Radiation scheme: 2 streams Wavelength: 280 - 700nm
Altitude: 118m
Date and time: 31.05.2018 12:00:00 respectively 20.12.2018 12:00:00
Latitude: 4.00937
Longitude: 8.404440
Solar zenith angle: 27.98776
Overhead ozone column: 300 du
Surface albedo: 0.1
Clouds: Opt. depth:0; Base:4; Top:5
Aerosols: Opt. depth: 0.235; S-S Alb: 0.99; Alpha: 1
Sunlight: Direct beam: 1; Diffuse down:1; Diffuse up:1

The calculated photolysis frequencies were used as a comparison for the NO₂-photolysis frequencies determined for the illumination conditions inside the AIDA-chamber.