

Supplement Information for:

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

Magdalena Vallon, Linyu Gao, Feng Jiang, Bianca Krumm, Jens Nadolny, Junwei Song, Thomas Leisner  
5 and Harald Saathoff

Institute of Meteorology and Climate Research, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen,  
Germany

*Correspondence to:* Harald.Saathoff ([Harald.Saathoff@kit.edu](mailto:Harald.Saathoff@kit.edu))

To be submitted to AMT special issue: ‘Simulation chambers as tools in atmospheric research’.

10 Table S1: Experimental conditions:

<b>Photolysis of 2,3-pentanedione</b>					
<b>starting concentration</b> <b>[ppb]</b>	<b>illumination</b> <b>[min]</b>	<b>relative humidity</b> <b>[%]</b>	<b>temperature</b> <b>[K]</b>		
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		

<b>Photolysis of DTDP</b>					
<b>DTDP</b>	<b>NH<sub>4</sub>NO<sub>3</sub></b> <b>[mol l<sup>-1</sup>]</b>	<b>(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub></b> <b>[mol l<sup>-1</sup>]</b>	<b>illumination</b> <b>[min]</b>	<b>relative humidity</b> <b>[%]</b>	<b>temperature</b> <b>[K]</b>
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 <sup>-1</sup>	0.025	0.009	120	79	293
1 ml of prepared DTDP solution	0.026	-	120	70	264

**Photosensitization experiments:**

Aerosol conc.	1 <sup>st</sup> illumination	2 <sup>nd</sup> illumination	relative humidity [%]	temperature
[ $\mu\text{g m}^{-3}$ ]	[min]	[min]	[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 <sup>-1</sup> ]	pinic acid [mol l <sup>-1</sup> ]	NH <sub>4</sub> NO <sub>3</sub> [mol l <sup>-1</sup> ]	Fe <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> (H <sub>2</sub> O) <sub>6</sub> [mol l <sup>-1</sup> ]	oxalic acid [mol l <sup>-1</sup> ]
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
--------	------------------------	-------	------	-----

15

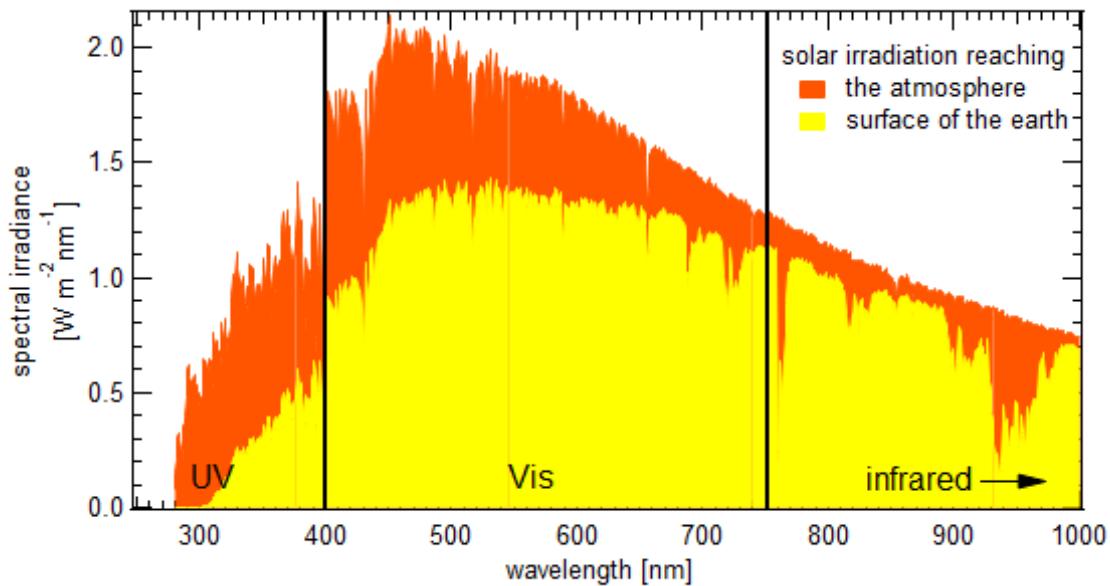


Figure S1: Solar Spectrum in the atmosphere derived from SMARTS v. 2.9.2 (ASTM G173-03 Reference Spectrum):

Reference: Data from United States Department of Energy, National Renewable Energy Laboratory, Reference Solar Spectral Irradiance: ASTM G-173, <https://www.nrel.gov/grid/solar-resource/assets/data/astmg173.xls>

20

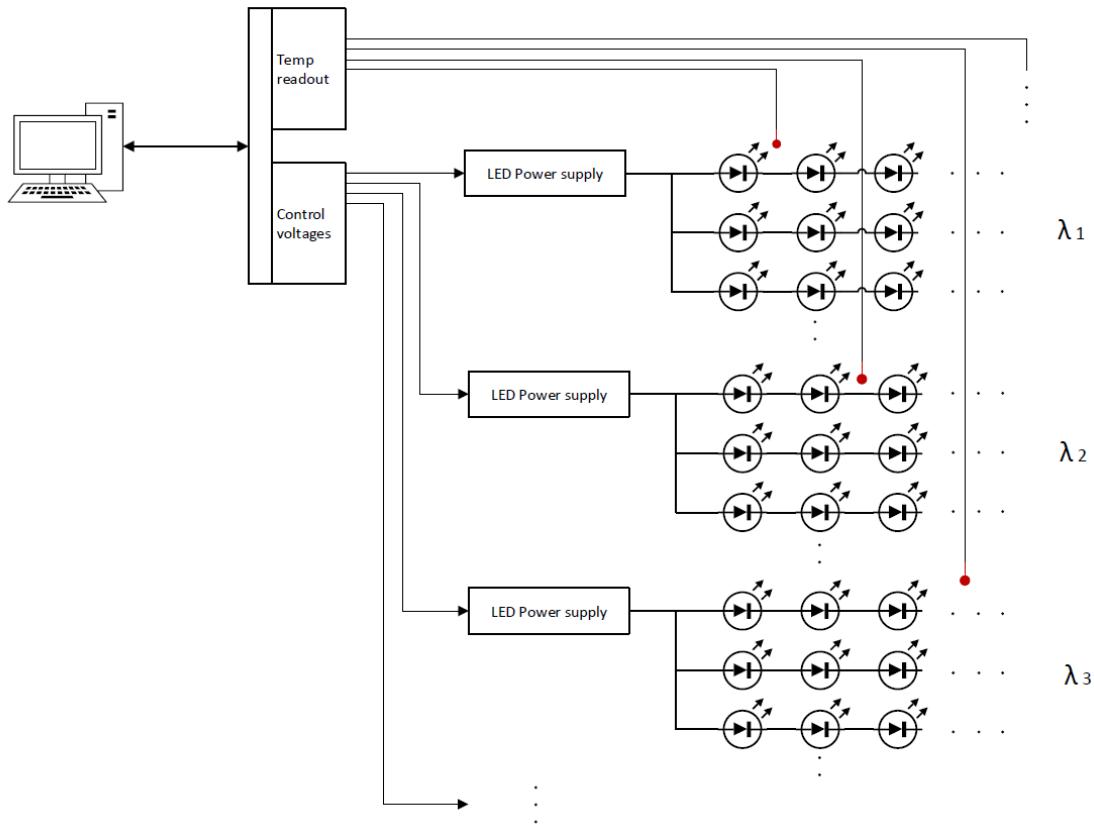
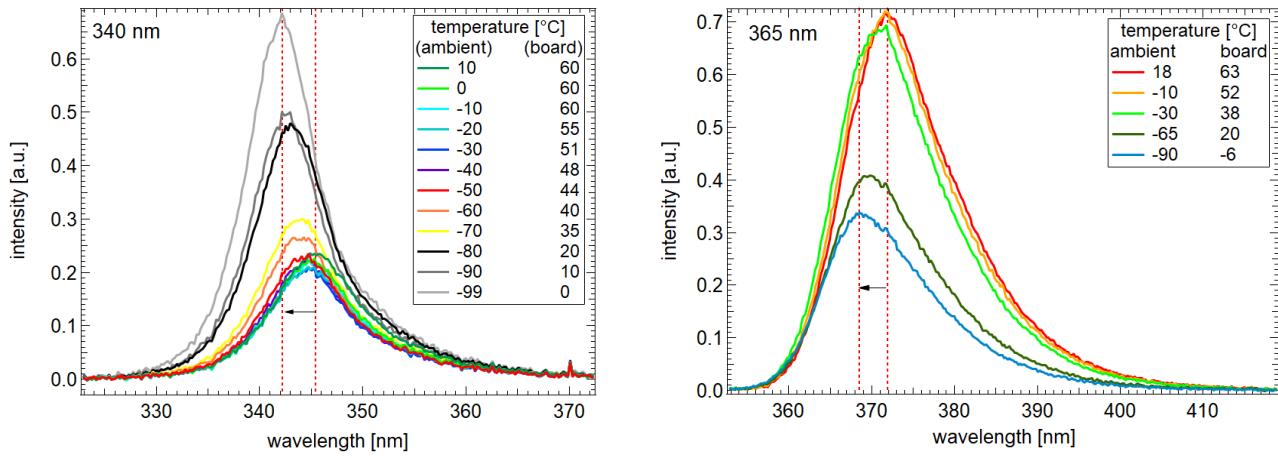


Figure S2: Electronic connection scheme for the LED power control and temperature readout.



25 Figure S3: 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.

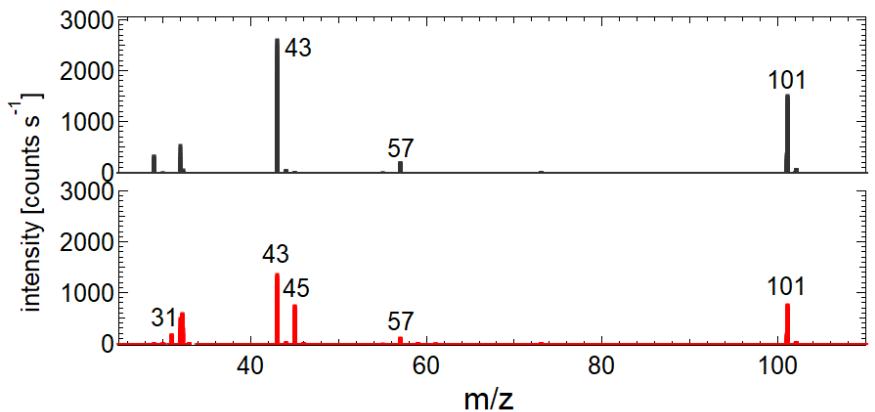


Figure S3: Mass Spectrum of 2,3-pentanedione before and after illumination (PTRMS): The mass peak for 2,3-pentanedione  
 30 can be found at m/z 101. M/z 43 and m/z 57 refer to fragments of 2,3-pentanedione. M/z 45 and m/z 31 refer to the reaction  
 products acetaldehyde and formaldehyde.

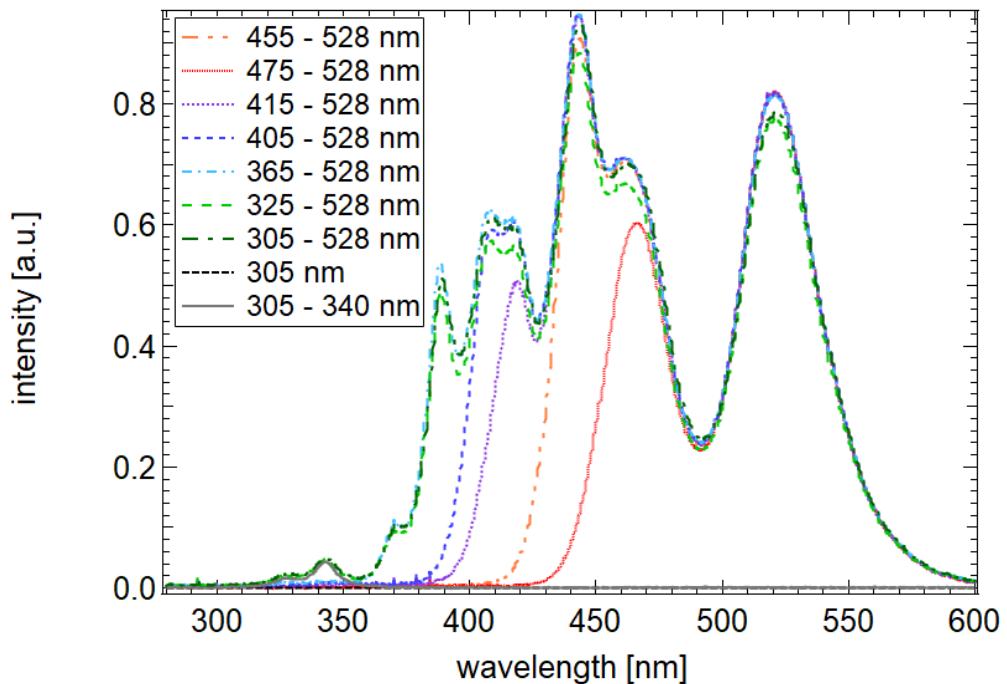


Figure S4: Spectra taken at the bottom of the chamber with different settings for the LEDs, resulting in different emission  
 35 spectra of the light source.

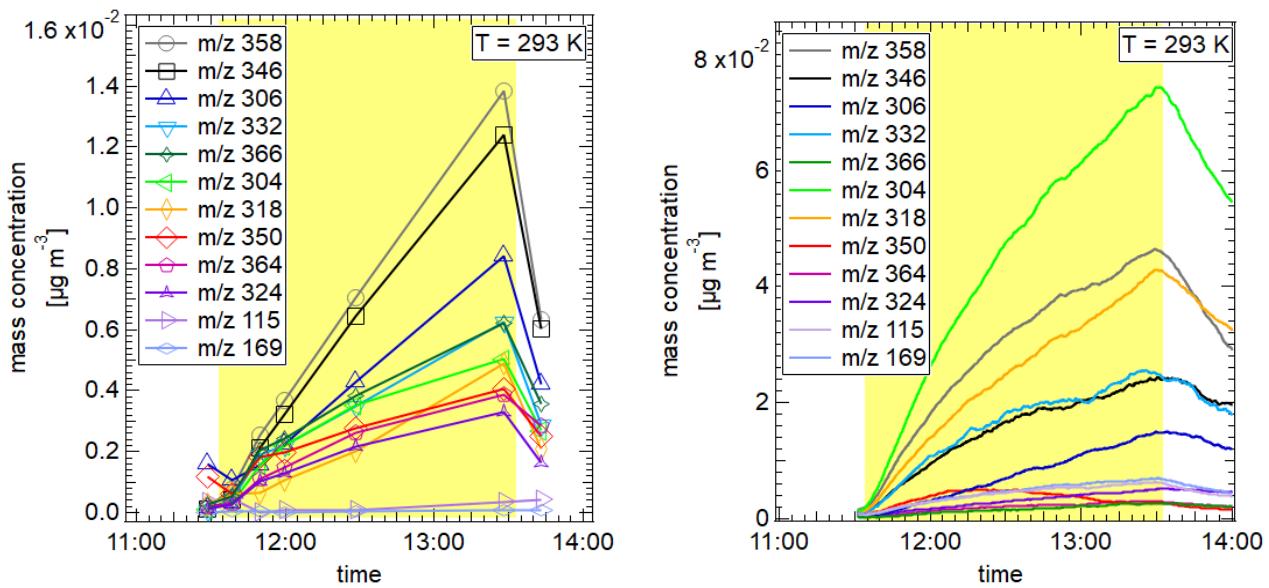


Figure S5: Mass increase of 16 components in particle (left) and gas phase (right) during illumination of an aerosol containing 3,5-diacetyl-2,4,6-trimethyl-1,4-dihydropyridine,  $(\text{NH}_4)_2\text{SO}_4$  and  $\text{NH}_4\text{NO}_3$ . The masses include the iodide used in the ionization process.

40

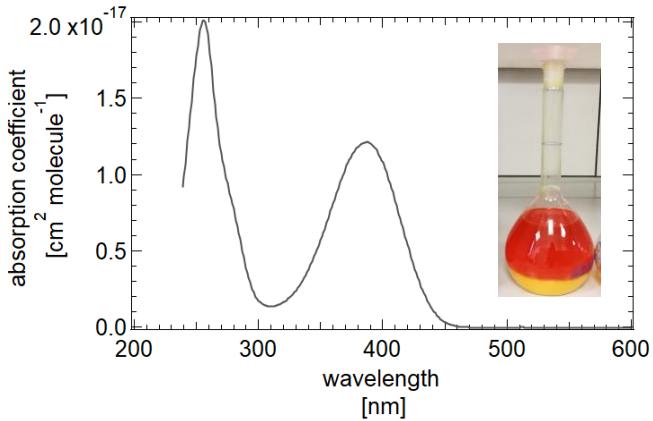
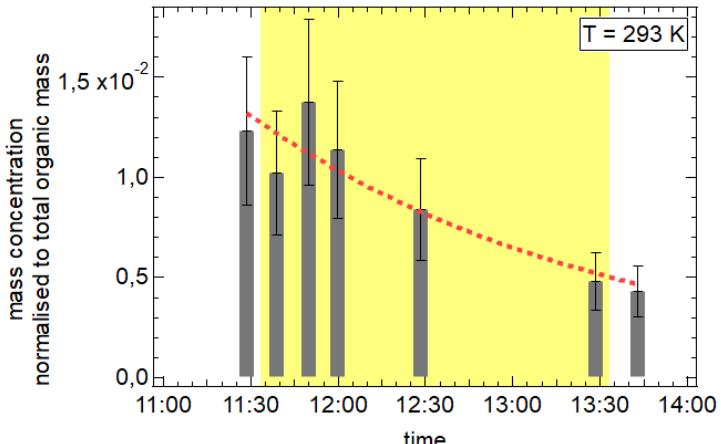
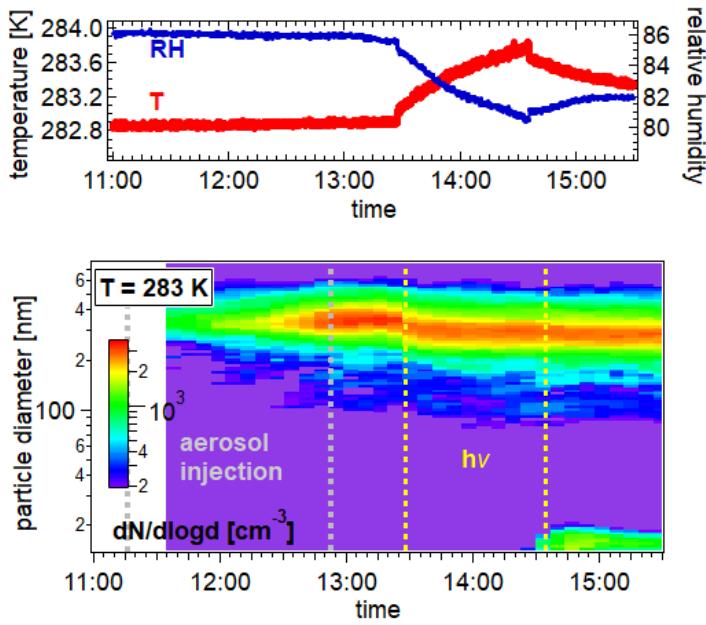


Figure S6: Absorption spectrum of 3,5-diacetyl-2,4,6-trimethyl-1,4-dihydropyridine ( $19.25 \mu\text{mol l}^{-1}$  in water). Insert shows the red colour of the compound in a mixture of water and methanol after synthesis from acetaldehyde and 2,3-pentadione in presence of  $(\text{NH}_4)_2\text{SO}_4$ .



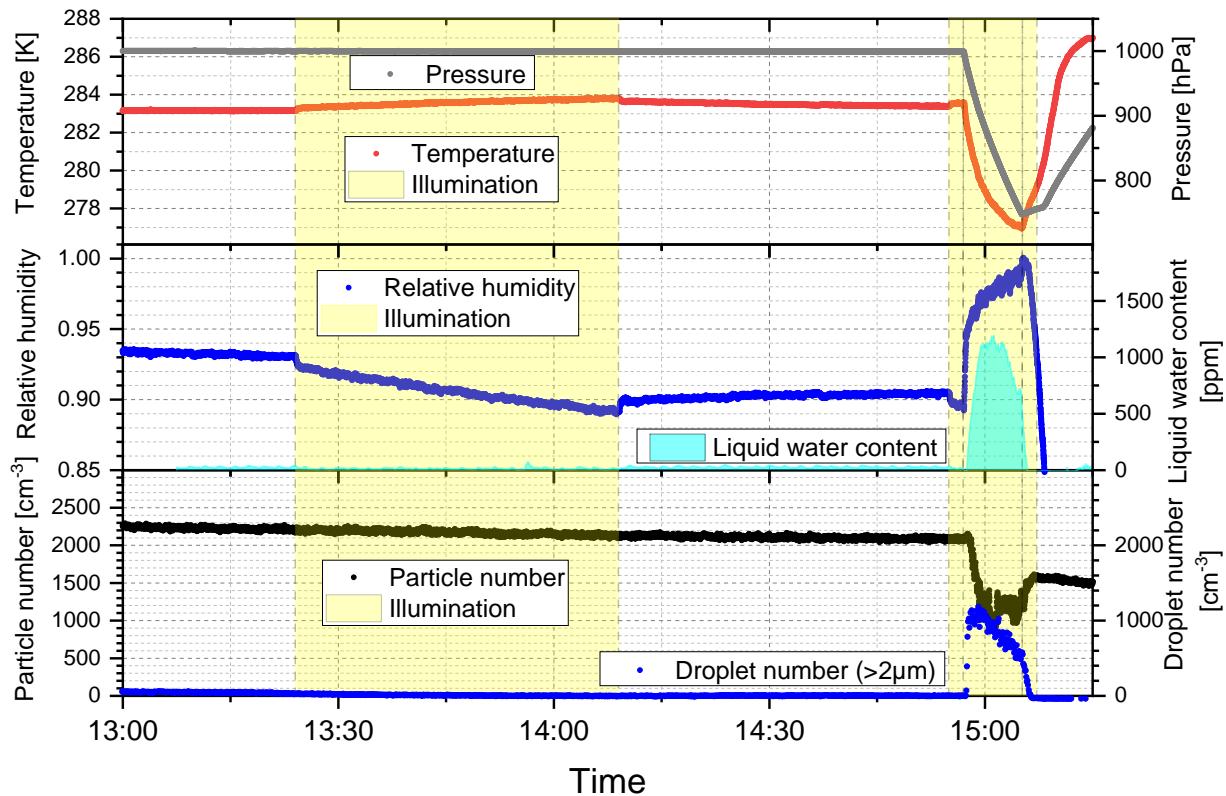
45

Figure S7: 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.



50

Figure S8: 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.



55 Figure S9: 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  
60 the temperature sensors and not to a real sudden change in temperature.

Text S1: NO<sub>2</sub>-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/](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

65

The calculated photolysis frequencies were used as a comparison for the NO<sub>2</sub>-photolysis frequencies determined for the illumination conditions inside the AIDA-chamber.