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Supplementary material

Photon flux dependence on solute environment in water ices

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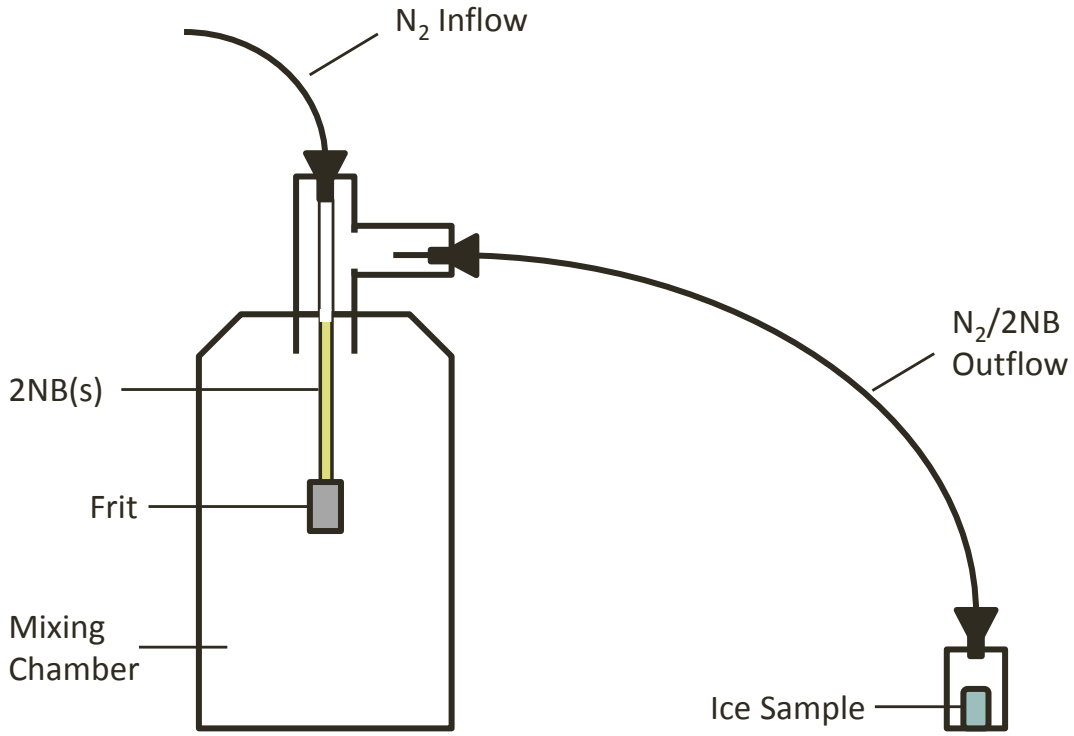

Fig. S1. Schematic of the gas deposition system used for surface deposition experiments. The system was preloaded with 0.4 g of solid 2NB and pure nitrogen (Praxair, 99.998 %) was passed through the system at a rate of 1.25 L min^{-1}, delivering a thawed sample equivalent of 1.0 μM 2NB s^{-1} for a volume of 1.0 mL. The chamber was covered in foil to prevent any NBA production from ambient light.

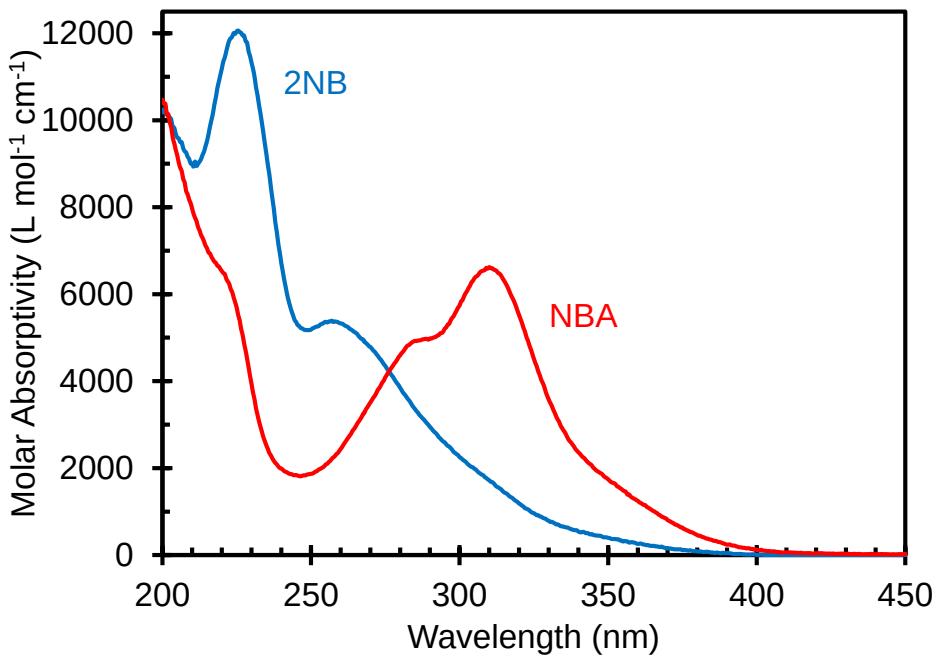

Fig. S2. Base-10 M absorptivities of 2NB and NBA. The 2NB result is from a 100-μM solution of 2NB prepared in Milli-Q water and measured in a Shimadzu UV2501PC spectrophotometer using a 1-cm quartz cuvette. The NBA result is from the same sample after simulated sunlight illumination for 35 min to completely convert the 2NB.

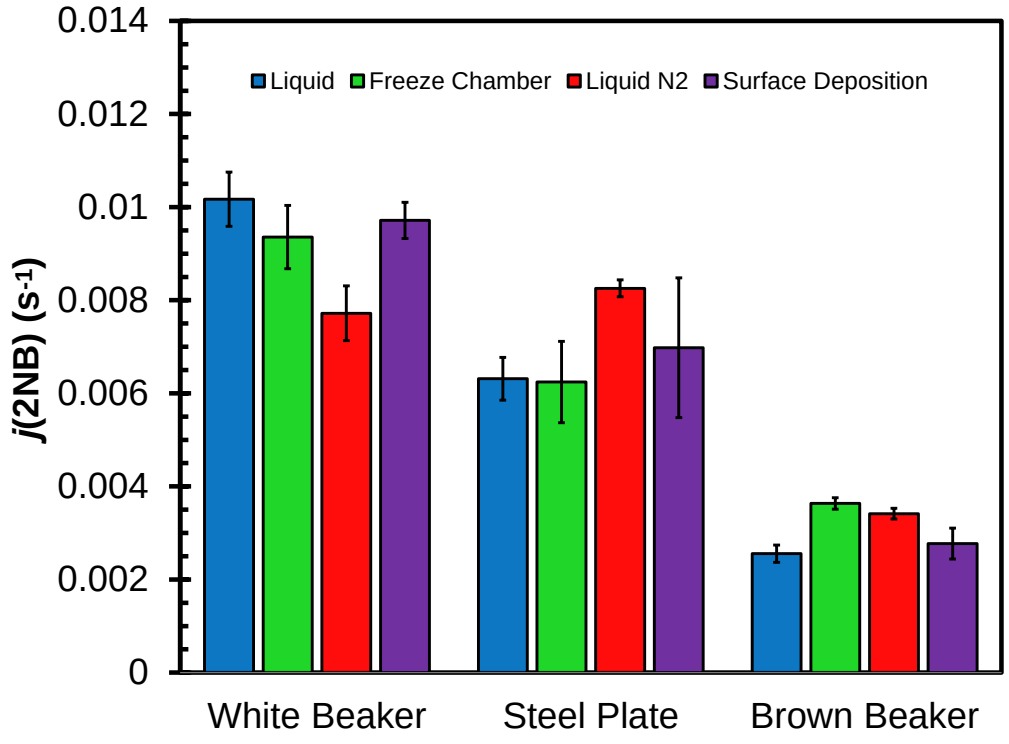

Fig. S3. Average *j*(2NB) values for liquid and ice experiments in each container type. Error bars represent ±1 σ.

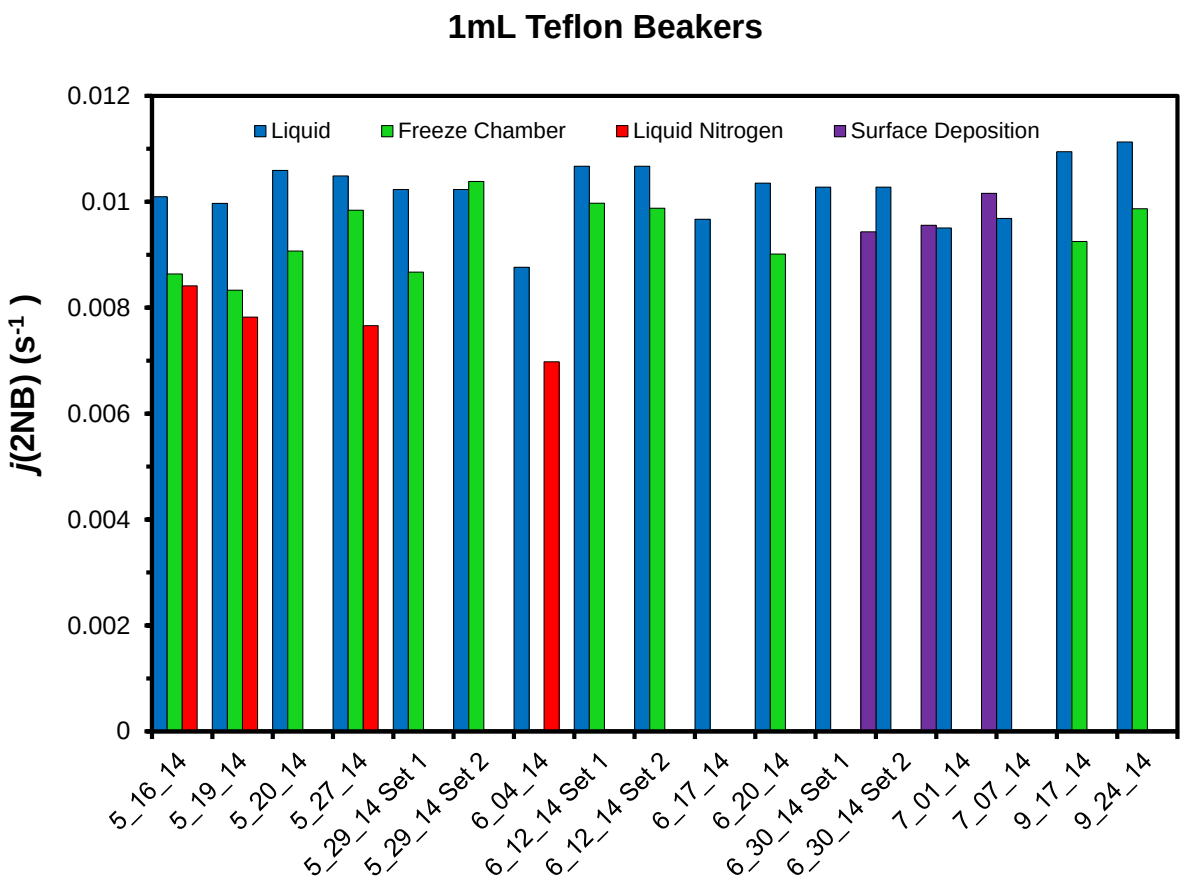

Fig. S4. Day-to-day variability in *j*(2NB) measurements for aqueous and ice experiments for one of the sample containers – 1-mL Teflon beakers.

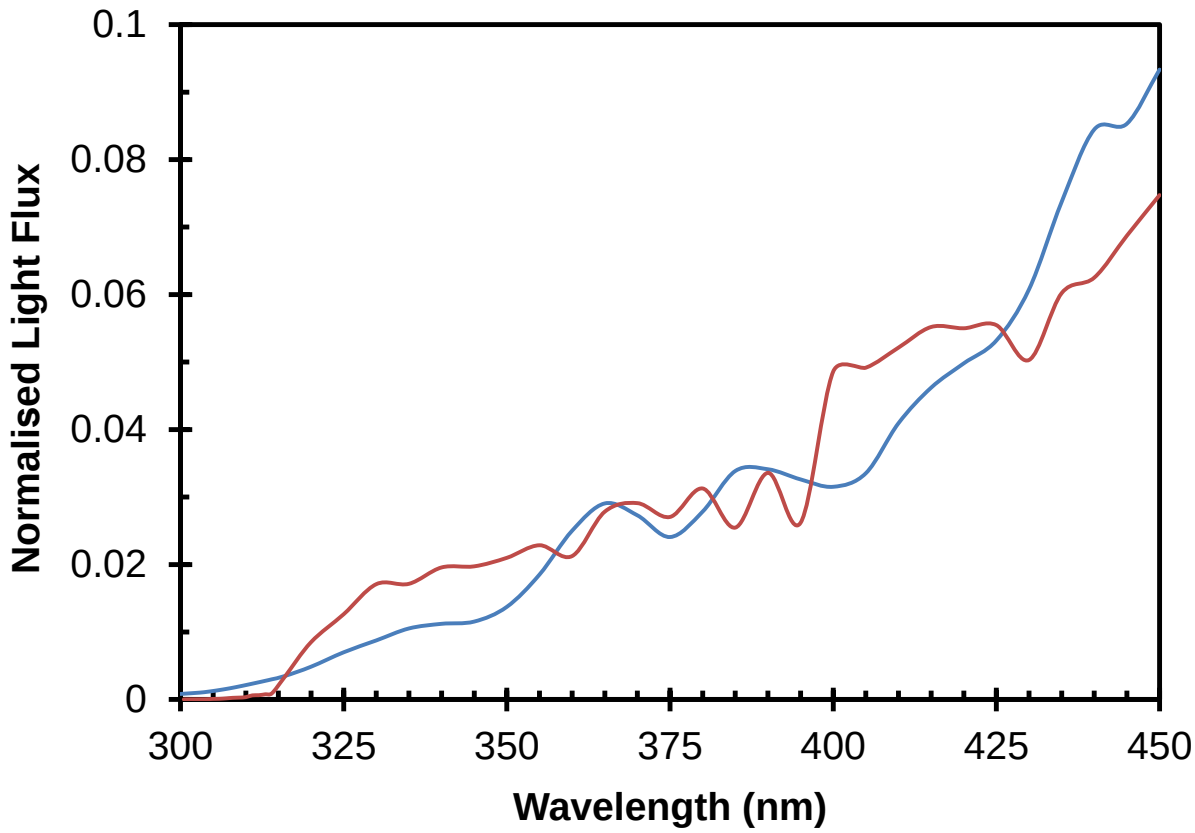

Fig. S5. Normalised light output of our illumination system compared with the normalised Tropospheric Ultraviolet and Visible (TUV) radiation model output for a solar zenith angle of 62°. Data was normalised such that the area under each curve was equal to 1.

Derivation of kinetic model for photoproduct quantitation

Because 2NB forms only one photoproduct (NBA), we can model the amount of photoproduct formed after a certain time *t* by simple manipulation of:

$$\frac{d[\mathrm{NBA}]}{dt} = j(2\mathrm{NB})[2\mathrm{NB}]_0 e^{-j(2\mathrm{NB})_t}$$

Integrating this equation, treating j(2NB) and $[2\mathrm{NB}]_0$ as constants of each experiment, we find

$$[\mathrm{NBA}]_t = [2\mathrm{NB}]_0 (1 - e^{-j(2\mathrm{NB})_t})$$

where $[\mathrm{NBA}]_t$ is the amount of photoproduct formed after a given time *t*.

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HPLC parameters

Manufacturer: Shimadzu

Liquid Chromatograph: LC-20AB

Autosampler: SFL-20A

Detector: SPD-M20A (photo diode array)

Column: Thermo Scientific BetaBasic 18, 250 × 3 mm, 5-µm grain size

Eluent: 60 : 40 acetonitrile : water, acidified to pH 2 with perchloric acid

Flow rate: 0.7 mL min^{-1}

Run time: 4.5 min

Table S1. Base-10 molar absorptivities for aqueous 2-nitrosobenzoic acid (NBA) at 298 K

Base-10 molar absorptivities (ε, M^{-1} cm^{-1}) were determined from the baseline-corrected absorbance of a single 100 µM 2NB aqueous solution allowed to undergo complete photodegradation (and conversion to NBA) under simulated sunlight (t = 35 min)

λ (nm)	ε	λ (nm)	ε	λ (nm)	ε	λ (nm)	ε
405	69	385	328	365	1004	345	1994
404	76	384	346	364	1050	344	2074
403	82	383	365	363	1091	343	2130
402	91	382	395	362	1137	342	2212
401	95	381	427	361	1181	341	2271
400	101	380	443	360	1230	340	2346
399	110	379	479	359	1272	339	2422
398	124	378	511	358	1309	338	2526
397	142	377	543	357	1380	337	2609
396	148	376	574	356	1436	336	2732
395	156	375	617	355	1471	335	2848
394	164	374	642	354	1523	334	2962
393	187	373	679	353	1565	333	3103
392	202	372	716	352	1636	332	3259
391	227	371	752	351	1663	331	3422
390	224	370	789	350	1726	330	3563
389	247	369	836	349	1775	329	3737
388	274	368	867	348	1844	328	3942
387	288	367	913	347	1886	327	4121
386	311	366	964	346	1929	326	4317

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λ (nm)	ε
325	4500
324	4714
323	4917
322	5125
321	5324
320	5509
319	5704
318	5869
317	6012
316	6168
315	6291
314	6408
313	6470
312	6538
311	6581
310	6605
309	6588
308	6527
307	6495
306	6407
305	6349
304	6252
303	6122
302	6001
301	5848
300	5722
299	5605
298	5477
297	5379
296	5281
295	5191
294	5091
293	5042

λ (nm)	ε
292	5001
291	4978
290	4967
289	4955
288	4947
287	4927
286	4917
285	4908
284	4875
283	4815
282	4761
281	4662
280	4578
279	4477
278	4383
277	4282
276	4187
275	4071
274	3952
273	3826
272	3711
271	3604
270	3494
269	3385
268	3266
267	3155
266	3050
265	2935
264	2842
263	2728
262	2630
261	2529
260	2425

λ (nm)	ε
259	2328
258	2257
257	2197
256	2124
255	2068
254	2001
253	1962
252	1914
251	1876
250	1852
249	1841
248	1817
247	1806
246	1802
245	1824
244	1826
243	1848
242	1884
241	1914
240	1974
239	2024
238	2104
237	2207
236	2329
235	2504
234	2692
233	2936
232	3212
231	3565
230	3919
229	4307
228	4689
227	5048

λ (nm)	ε
226	5383
225	5675
224	5904
223	6099
222	6276
221	6445
220	6515
219	6619
218	6703
217	6786
216	6918
215	7042
214	7196
213	7344
212	7526
211	7737
210	7953
209	8157
208	8352
207	8636
206	8890
205	9176
204	9454
203	9814
202	10122
201	10362
200	10454