Supplement of Atmos. Chem. Phys. Discuss., 14, 20585–20615, 2014
http://www.atmos-chem-phys-discuss.net/14/20585/2014/
doi:10.5194/acpd-14-20585-2014-supplement

Atmospheric Chemistry and Physics Discussions

Supplement of

Ultraviolet and visible complex refractive indices of secondary organic material produced by photooxidation of the aromatic compounds toluene and *m*-Xylene

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Supporting Information

Ultraviolet and Visible Complex Refractive Indices of Secondary Organic Material Produced by Photooxidation of the Aromatic Compounds Toluene and *m*-Xylene

by

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Submitted: July 2014

Atmospheric Chemistry and Physics

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S1. Imaginary refractive indices *k* of nitro-aromatics

Figure S1 shows the imaginary refractive indices *k* for several different pure compounds relevant to nitrogen-containing species present in SOM produced from aromatic precursors. Compounds were commercially available and used without further purification (2-methyl-4-nitrophenol, Sigma Aldrich, 97%; 4-methyl-2-nitrophenol, Sigma Aldrich, 99%; 4-methyl-3-nitrophenol, Sigma Aldrich, 97%; 2,4-dimethyl-6-nitrophenol, Tokyo Chemical Industry Co. Ltd, 98%). The *k* values were calculated using Eq. 1. The results confirm that nitro-aromatic compounds are strong UV-absorbers. In particular, the aromatic compounds having hydroxyl and nitro groups in *para* substitution, such as 2-methyl-4-nitrophenol, have a strong absorption band at 320 nm. Compounds having this configuration possibly contribute to the main observed absorption (Fig. 2b). This result is consistent with the findings of Nakayama et al. (2013).

S2. Infrared absorption bands and the ternary diagram

The infrared absorption bands and quantification windows of organic functional groups are listed in Table S1. For an infrared spectrum, the peak areas *A* of O–H (including O–H in alcohol, phenol, and carboxylic acid), C–O, and C=O were determined by the band fitting algorithm described in section 2.4. Three variables representing relative areas of O–H, C–O, and C=O absorption bands are defined as follows.

$$a = A_{\text{O-H}} / (A_{\text{O-H}} + A_{\text{C-O}} + A_{\text{C=O}})$$

$$b = A_{\text{C-O}} / (A_{\text{O-H}} + A_{\text{C-O}} + A_{\text{C=O}})$$

$$c = A_{\text{C=O}} / (A_{\text{O-H}} + A_{\text{C-O}} + A_{\text{C=O}})$$

These three variables *a*, *b*, and *c* sum to unity. A ternary diagram can be created using those three variables, as shown in Fig. S2. The three different types of oxygenated bonding (i.e., O–H, C–O, and C=O) are denoted at the vertices of the triangle. The position of the infrared spectrum with

relative areas of *a*, *b* and *c* are denoted as point *X*. From the ternary diagram, the relative abundances of O–H, C–O, and C=O are depicted.

References

Nakayama, T., Sato, K., Matsumi, Y., Imamura, T., Yamazaki, A., and Uchiyama, A.: Wavelength and NOx dependent complex refractive index of SOAs generated from the photooxidation of toluene, Atmos. Chem. Phys., 13, 531-545, 10.5194/acp-13-531-2013, 2013.

Table S1. Absorptive component *k* of the refractive indices of toluene- and *m*-xylene-derived SOMs for several different initial NO concentrations. See Table 1 for experimental conditions.

SOM type:	Toluene-derived SOM				*m*-Xylene-derived SOM			
wavelength (nm)	A1	A2	A3	A4	B1	B2	B3	B4
280	0.0262	0.0326	0.0365	0.0400	0.0267	0.0261	0.0268	0.0265
285	0.0241	0.0309	0.0349	0.0387	0.0245	0.0242	0.0250	0.0252
290	0.0217	0.0291	0.0332	0.0373	0.0215	0.0217	0.0226	0.0235
295	0.0193	0.0275	0.0315	0.0361	0.0179	0.0187	0.0197	0.0214
300	0.0171	0.0261	0.0301	0.0351	0.0143	0.0159	0.0169	0.0193
305	0.0153	0.0249	0.0289	0.0343	0.0115	0.0137	0.0147	0.0176
310	0.0137	0.0238	0.0279	0.0337	0.0095	0.0121	0.0131	0.0163
315	0.0124	0.0228	0.0270	0.0333	0.0081	0.0110	0.0120	0.0153
320	0.0114	0.0217	0.0259	0.0327	0.0071	0.0101	0.0112	0.0146
325	0.0104	0.0204	0.0247	0.0320	0.0063	0.0093	0.0104	0.0139
330	0.0094	0.0191	0.0233	0.0312	0.0056	0.0086	0.0097	0.0133
335	0.0086	0.0175	0.0219	0.0302	0.0049	0.0078	0.0089	0.0125
340	0.0077	0.0160	0.0203	0.0290	0.0044	0.0071	0.0082	0.0117
345	0.0069	0.0145	0.0188	0.0277	0.0038	0.0064	0.0074	0.0108
350	0.0062	0.0132	0.0173	0.0263	0.0034	0.0057	0.0066	0.0099
355	0.0055	0.0119	0.0158	0.0247	0.0030	0.0051	0.0059	0.0090
360	0.0050	0.0107	0.0146	0.0234	0.0027	0.0045	0.0053	0.0083
365	0.0044	0.0096	0.0132	0.0219	0.0023	0.0039	0.0047	0.0074
370	0.0039	0.0086	0.0120	0.0206	0.0020	0.0034	0.0041	0.0067
375	0.0035	0.0077	0.0109	0.0195	0.0018	0.0029	0.0037	0.0060
380	0.0031	0.0069	0.0100	0.0187	0.0016	0.0026	0.0032	0.0054
385	0.0027	0.0062	0.0091	0.0178	0.0014	0.0022	0.0028	0.0049
390	0.0024	0.0056	0.0083	0.0169	0.0012	0.0019	0.0025	0.0044
395	0.0022	0.0050	0.0077	0.0163	0.0010	0.0016	0.0021	0.0039
400	0.0020	0.0046	0.0071	0.0158	0.0009	0.0014	0.0018	0.0034
405	0.0017	0.0041	0.0066	0.0153	0.0008	0.0012	0.0016	0.0030
410	0.0016	0.0037	0.0060	0.0144	0.0007	0.0010	0.0014	0.0026
415	0.0014	0.0034	0.0056	0.0139	0.0006	0.0008	0.0012	0.0023
420	0.0013	0.0031	0.0052	0.0134	0.0006	0.0007	0.0010	0.0021
425	0.0012	0.0028	0.0048	0.0129	0.0005	0.0006	0.0008	0.0018
430	0.0011	0.0026	0.0047	0.0126	0.0005	0.0005	0.0007	0.0016
435	0.0010	0.0023	0.0041	0.0116	0.0005	0.0005	0.0006	0.0014
440	0.0010	0.0021	0.0038	0.0113	0.0004	0.0004	0.0005	0.0012
445	0.0009	0.0019	0.0035	0.0107	0.0004	0.0004	0.0004	0.0011
450	0.0008	0.0016	0.0031	0.0098	0.0004	0.0003	0.0004	0.0009
455	0.0008	0.0014	0.0027	0.0089	0.0003	0.0002	0.0003	0.0009
460	0.0008	0.0012	0.0025	0.0081	0.0003	0.0002	0.0002	0.0007

465	0.0008	0.0011	0.0022	0.0075	0.0003	0.0002	0.0002	0.0007
470	0.0007	0.0008	0.0017	0.0063	0.0002	0.0001	0.0002	0.0006
475	0.0007	0.0007	0.0015	0.0059	0.0002	0.0001	0.0001	0.0005
480	0.0007	0.0006	0.0013	0.0054	0.0002	0.0001	0.0001	0.0004
485	0.0007	0.0004	0.0012	0.0053	0.0002	0.0000	0.0002	0.0004
490	0.0006	0.0003	0.0010	0.0045	0.0002	0.0000	0.0000	0.0003
495	0.0005	0.0002	0.0007	0.0039	0.0002	0.0000	0.0000	0.0003
500	0.0006	0.0001	0.0006	0.0034	0.0001	0.0000	0.0000	0.0003
505	0.0005	0.0000	0.0004	0.0029	0.0001	0.0000	0.0000	0.0002
510	0.0005	0.0000	0.0003	0.0023	0.0001	0.0000	0.0000	0.0002
515	0.0004	0.0000	0.0001	0.0017	0.0001	0.0000	0.0000	0.0002
520	0.0004	0.0000	0.0000	0.0013	0.0001	0.0000	0.0000	0.0001
525	0.0004	0.0000	0.0000	0.0010	0.0001	0.0000	0.0000	0.0001
530	0.0003	0.0000	0.0000	0.0008	0.0001	0.0000	0.0000	0.0001
535	0.0003	0.0000	0.0000	0.0007	0.0001	0.0000	0.0000	0.0001
540	0.0004	0.0000	0.0000	0.0005	0.0001	0.0000	0.0000	0.0001
545	0.0003	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0001
550	0.0003	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0001
555	0.0003	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0001
560	0.0003	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0001

Table S2. Parameters for Cauchy's equation[a] to describe the wavelength-dependent real refractive index *n* of toluene- and *m*-xylene-derived SOMs for several initial NO concentrations.[b]

	Precursor	NO_0 (ppm)	*B*	*C* (μm^2)	*D* (μm^4)
A1	Toluene	0.0	1.505	7.57×10^{-3}	-1.17×10^{-4}
A2	Toluene	2.5	1.514	6.87×10^{-3}	-1.16×10^{-4}
A3	Toluene	5.0	1.513	9.07×10^{-3}	-1.72×10^{-4}
A4	Toluene	10.0	1.519	1.03×10^{-2}	-2.91×10^{-4}
B1	*m*-Xylene	0.0	1.499	4.59×10^{-3}	9.84×10^{-5}
B2	*m*-Xylene	2.5	1.500	5.53×10^{-3}	3.63×10^{-5}
B3	*m*-Xylene	5.0	1.501	7.77×10^{-3}	1.45×10^{-5}
B4	*m*-Xylene	10.0	1.510	1.07×10^{-2}	-2.60×10^{-4}

[a]Cauchy's equation: $n(\lambda) = B + C/\lambda^2 + D/\lambda^4$.

[b]Range of applicability is for 280 to 1200 nm.

Table S3. Absorption ranges of organic functional groups and quantification windows used in the analysis

Functional groups	Absorption range (cm^{-1})	Quantification window (cm^{-1})
Alkane C–H	2700-3000	2790-2980
Alcohol (including phenol) O–H	3100-3700	3200-3600
Carboxylic acid O–H	2400-3300	2600-3100
Carbonyl C=O	1640-1850	1728
C–O	900-1260	1000-1260
Nitrate $–ONO_2$	846, 1281, and 1647	1647
Nitro $–NO_2$	1558 and 1342	1558

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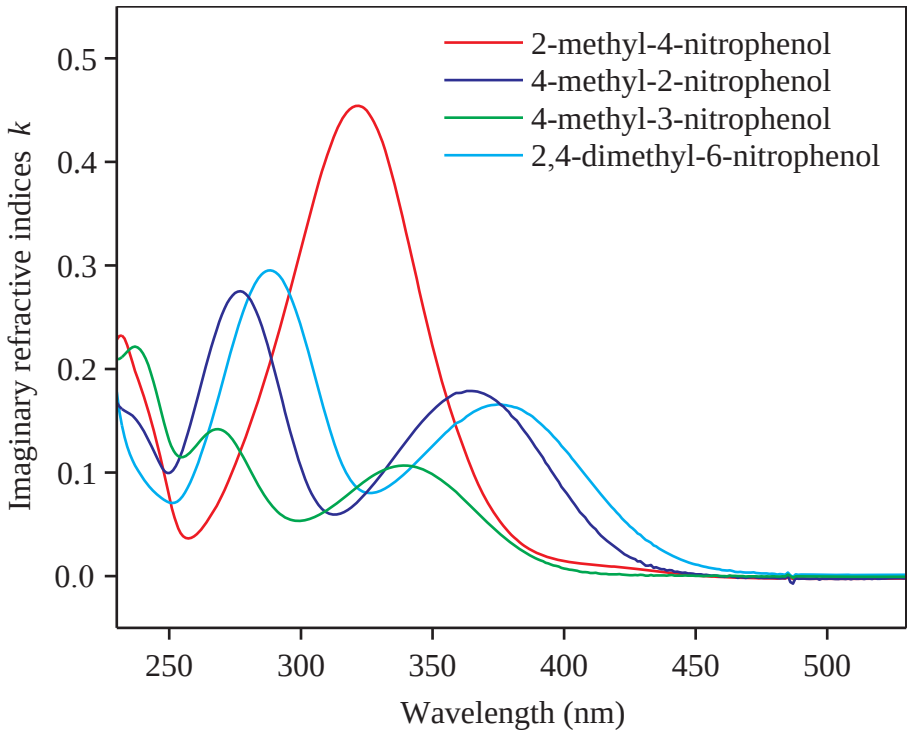
2-methyl-4-nitrophenol
4-methyl-2-nitrophenol
4-methyl-3-nitrophenol
2,4-dimethyl-6-nitrophenol
Imaginary refractive indices k
0.0
0.1
0.2
0.3
0.4
0.5
250
300
350
400
450
500
Wavelength (nm)

Figure S1

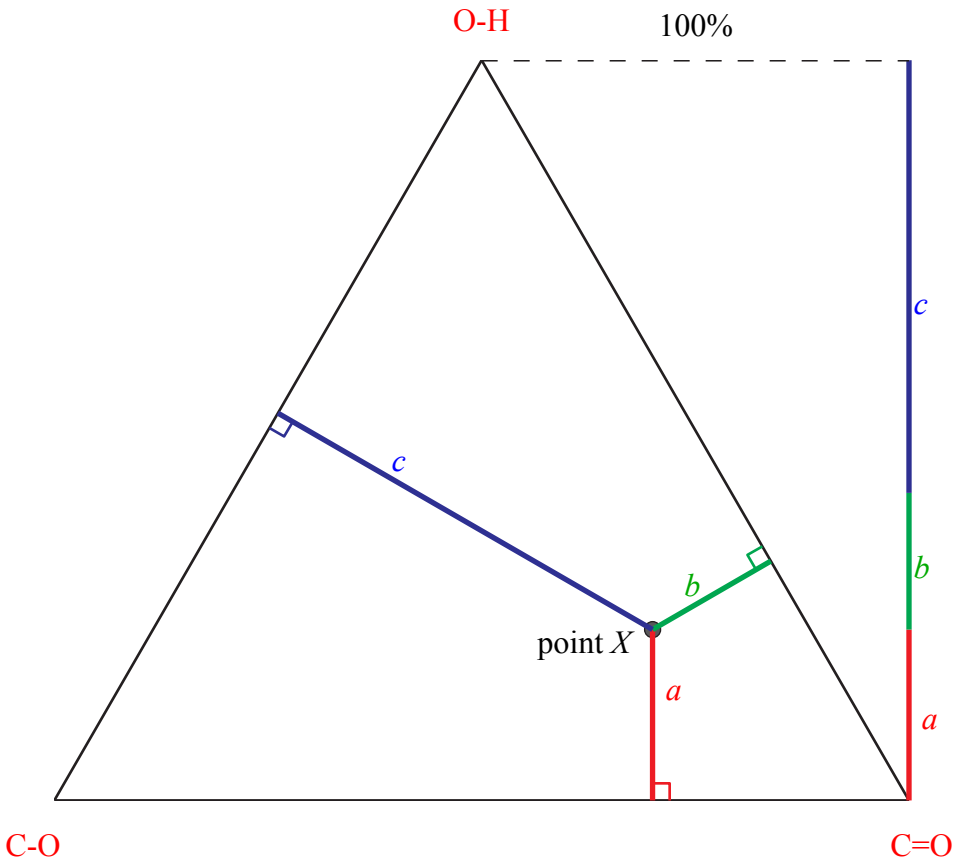

Figure S2