

Supplementary material of

**Anthropogenic VOC in Abidjan, southern West Africa: from source quantification to atmospheric impacts**

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Table S1. Mean VOC to CO emission ratios (ERs, ppbv per ppmv CO) for each emission source analysed in this study.

	MW (g mol <sup>-1</sup> )	SOAP value	kOH value	Mean ER VOC/CO ± SD (ppbv/ppmv)									
				HDDV	TW 2T	TW 4T	CH	FW	CHM	WB	LDDV	LDGV	HDDV-T
benzene	78.11	92.9	1.2	0.42 ± 0.03	53.2 ± 10.7	10.5 ± 4.17	1.76 ± 1.80	1.51	0.94	12.75 ± 8.43	3.06 ± 1.17	1.41 ± 0.25	13.74
toluene	92.14	100	5.6	0.26 ± 0.05	117.6 ± 25	15.9 ± 4.33	0.58 ± 0.43	0.83	0.67	18.1 ± 14.6	1.21 ± 0.57	6.90 ± 3.16	4.62
m+p-xylene	106.16	76.3	19	0.21 ± 0.04	102.1 ± 10	8.32 ± 3.77	0.32 ± 0.18	0.58	0.27	1.96 ± 2.22	0.33 ± 0.04	10.0 ± 0.86	3.26
o-xylene	106.16	95.5	14	0.08 ± 0.02	58.3 ± 15.7	3.22 ± 1.32	0.08 ± 0.06	0.06	0.08	0.03 ± 0.04	0.17 ± 0.05	4.82 ± 1.03	1.08
ethylbenzene	106.17	111.6	7.5	0.07 ± 0.02	59.5 ± 15.9	5.57 ± 2.55	0.29 ± 0.32	0.10	0.09	11.66 ± 8.3	0.25 ± 0.08	2.53 ± 0.75	1.26
styrene	104.15	212.3	43	0.06 ± 0.01	37.5 ± 23.8	2.79 ± 2.03	2.79 ± 0.09	0.16	0.16	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.05
iso-propylbenzene	120.19	95.5	6.6	0.01 ± 0.01	8.32 ± 1.87	0.62 ± 0.43	n.d.	0.01	0.01	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.44
1,3,5-trimethylbenzene	120.19	13.5	60	0.06 ± 0.01	30.1 ± 13.0	0.83 ± 0.35	0.00 ± 0.00	0.02	0.04	0.56 ± 0.57	0.13 ± 0.01	1.32 ± 0.07	0.90
1,2,4-trimethylbenzene	120.19	20.6	32	0.19 ± 0.04	65.6 ± 24.5	2.83 ± 1.25	0.02 ± 0.01	0.02	0.10	0.49 ± 0.41	0.42 ± 0.02	4.29 ± 0.54	4.17
1,2,3-trimethylbenzene	120.19	43.9	29	0.07 ± 0.01	20.8 ± 7.58	0.62 ± 0.27	0.65 ± 0.85	0.21	0.14	0.16 ± 0.15	0.17 ± 0.01	0.73 ± 0.12	1.64
isoprene	68.12	1.9	100	0.02 ± 0.01	3.99 ± 1.88	0.68 ± 0.24	0.07 ± 0.04	1.68	0.22	2.08 ± 2.84	0.04 ± 0.04	0.17 ± 0.15	0.29
hexene	84.16	0	37	n.d.	22.7 ± 6.44	0.35 ± 0.28	0.35 ± 0.11	0.00	0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	1.06
pentane	72.15	0.3	3.8	0.01 ± 0.00	42.6 ± 8.85	3.50 ± 0.55	3.50 ± 0.13	0.07	0.07	n.d.	n.d.	n.d.	0.09
2-methylpentane	86.18	0	5.2	0.02 ± 0.01	73.5 ± 0.43	5.91 ± 4.28	5.91 ± 2.26	0.00	0.00	n.d.	n.d.	n.d.	0.49
3-methylpentane <sup>2</sup>	86.18	0.2	5.2	0.01 ± 0.00	61.2 ± 14.9	3.53 ± 2.48	3.53 ± 3.44	0.42	0.42	n.d.	n.d.	n.d.	0.00
hexane	86.18	0.1	5.2	0.02 ± 0.00	75.1 ± 3.90	5.82 ± 4.21	5.82 ± 1.21	0.01	0.01	n.d.	n.d.	n.d.	0.06
2,2-dimethylpentane	100.21	0	4.77	0.00 ± 0.00	7.21 ± 1.95	0.12 ± 0.09	0.12 ± 0.01	0.16	0.16	n.d.	n.d.	n.d.	0.43
2,4-dimethylpentane <sup>1,2</sup>	100.21	0.3	4.77	0.00 ± 0.00	24.3 ± 2.70	0.38 ± 0.27	0.38 ± 0.02	0.02	0.02	n.d.	n.d.	n.d.	0.00
2,2,3-trimethylbutane <sup>1</sup>	100.21	0.3	3.81	0.00 ± 0.00	3.07 ± 0.89	0.06 ± 0.05	0.06 ± 0.01	0.02	0.02	n.d.	n.d.	n.d.	0.06
3,3-dimethylpentane <sup>1,2</sup>	100.21	0.3	4.77	0.01 ± 0.00	8.45 ± 1.75	0.02 ± 0.01	0.02 ± 0.00	0.21	0.21	n.d.	n.d.	n.d.	0.13
cyclohexane	84.16	1	7	0.00 ± 0.00	26.6 ± 15.8	1.66 ± 1.09	1.66 ± 0.35	0.01	0.01	n.d.	n.d.	n.d.	0.05
2-methylhexane <sup>2</sup>	100.21	0	7	0.01 ± 0.00	68.4 ± 14.4	1.81 ± 1.31	1.81 ± 0.00	0.05	0.05	n.d.	n.d.	n.d.	0.17
2,3-dimethylpentane <sup>2</sup>	100.21	0.4	4.77	n.d.	20.6 ± 10.9	0.55 ± 0.40	0.55 ± 0.00	0.00	0.00	n.d.	n.d.	n.d.	0.01
heptane	100.21	0.1	6.8	0.13 ± 0.07	40.0 ± 13.1	2.34 ± 1.17	0.09 ± 0.05	0.02	0.53	3.09 ± 3.40	0.06 ± 0.04	0.08 ± 0.04	0.29
octane	114.23	0.8	8.1	0.25 ± 0.12	32.1 ± 13.1	0.94 ± 0.48	0.10 ± 0.05	0.84	0.20	2.02 ± 1.95	0.05 ± 0.02	0.33 ± 0.09	0.89
iso-octane	114.23	0.8	3.34	0.03 ± 0.02	16.8 ± 6.49	0.15 ± 0.05	0.04 ± 0.04	0.13	0.01	0.12 ± 0.13	0.05 ± 0.03	0.01 ± 0.00	0.25
nonane	128.26	1.9	9.7	0.14 ± 0.03	10.6 ± 7.36	0.32 ± 0.23	0.32 ± 0.00	0.02	0.02	n.d.	n.d.	n.d.	3.71
decane	142.29	7	11	0.24 ± 0.06	6.66 ± 3.49	0.15 ± 0.10	0.15 ± 0.02	0.00	0.00	n.d.	n.d.	n.d.	8.26

	MW (g mol <sup>-1</sup> )	SOAP value	<i>k</i> OH value	Mean ER VOC/CO ± SD (ppbv/ppmv)									
				HDDV	TW 2T	TW 4T	CH	FW	CHM	WB	LDDV	LDGV	HDDV-T
undecane	156.31	16.2	12	0.28 ± 0.02	2.05 ± 1.71	0.06 ± 0.04	0.06 ± 0.05	0.00	0.00	n.d.	n.d.	n.d.	0.62
dodecane	170.33	34.5	13.2	0.28 ± 0.02	1.01 ± 1.05	0.03 ± 0.02	0.03 ± 0.00	0.01	0.01	n.d.	n.d.	n.d.	14.72
tridecane <sup>1</sup>	184.36	34.5	15.1	0.02 ± 0.00	0.08 ± 0.05	0.00 ± 0.00	0.00 ± 0.00	0.00	0.00	n.d.	n.d.	n.d.	0.17
tetradecane <sup>1</sup>	198.39	34.5	17.9	0.06 ± 0.01	0.24 ± 0.18	0.01 ± 0.00	0.01 ± 0.00	0.01	0.01	n.d.	n.d.	n.d.	2.19
pentadecane <sup>1</sup>	212.41	34.5	20.7	0.02 ± 0.00	0.08 ± 0.08	0.00 ± 0.00	0.00 ± 0.00	0.04	0.04	n.d.	n.d.	n.d.	1.23
hexadecane <sup>1</sup>	226.44	34.5	23.2	0.02 ± 0.00	0.08 ± 0.03	0.00 ± 0.00	0.00 ± 0.00	0.01	0.01	n.d.	n.d.	n.d.	0.85
limonene	136.24	18	164	0.01 ± 0.00	0.41 ± 0.30	0.00 ± 0.00	0.02 ± 0.02	0.47	0.03	10.83 ± 7.9	0.00 ± 0.00	0.00 ± 0.00	0.49
α-pinene	136.23	17.4	52.3	0.01 ± 0.00	1.81 ± 0.73	0.01 ± 0.01	0.05 ± 0.07	0.00	0.00	0.02 ± 0.02	0.00 ± 0.00	0.00 ± 0.00	0.26
β-pinene	136.23	18.1	74.3	0.02 ± 0.01	0.93 ± 0.59	0.01 ± 0.00	0.06 ± 0.09	0.01	0.00	0.20 ± 0.19	0.00 ± 0.00	0.00 ± 0.00	0.28
camphene <sup>1</sup>	136.24	18	53	0.06 ± 0.02	0.34 ± 0.31	0.01 ± 0.01	0.01 ± 0.00	0.00	0.00	n.d.	n.d.	n.d.	0.36
myrcene <sup>1</sup>	136.23	18	215	0.00 ± 0.00	0.65 ± 0.41	0.00 ± 0.00	0.00 ± 0.01	0.01	0.01	n.d.	n.d.	n.d.	0.37
3-carene <sup>1</sup>	136.24	18	85	0.00 ± 0.00	0.41 ± 0.45	0.01 ± 0.01	0.01 ± n.d.	0.00	0.00	n.d.	n.d.	n.d.	0.39
α-terpinene <sup>1</sup>	136.23	18	363	0.02 ± 0.01	4.15 ± 2.45	0.19 ± 0.13	0.19 ± 0.00	0.00	0.00	n.d.	n.d.	n.d.	1.05
α-ocimene <sup>1</sup>	136.23	18	252	0.02 ± 0.00	12.3 ± 4.10	0.31 ± 0.17	0.31 ± 0.00	0.01	0.01	n.d.	n.d.	n.d.	3.62
γ-terpinene <sup>1</sup>	136.23	18	177	0.05 ± 0.00	0.96 ± 0.75	0.01 ± 0.01	0.01 ± 0.00	0.09	0.09	n.d.	n.d.	n.d.	0.33
terpinolene <sup>1</sup>	136.24	18	225	0.00 ± 0.00	0.62 ± 0.35	0.03 ± 0.03	0.03 ± 0.00	0.01	0.01	n.d.	n.d.	n.d.	0.19
hexanal	100.16	0	30	0.00 ± 0.00	14.2 ± 14.2	0.03 ± 0.03	0.03 ± 0.00	0.05	0.05	n.d.	n.d.	n.d.	0.14
heptanal <sup>1,2</sup>	114.19	0	30	0.01 ± 0.00	n.d.	n.d.	n.d.	0.01	0.01	n.d.	n.d.	n.d.	0.60
benzaldehyde	106.12	216.1	12	0.03 ± 0.03	5.78 ± 4.43	0.10 ± 0.08	0.10 ± n.d.	0.00	0.00	n.d.	n.d.	n.d.	0.01
octanal <sup>1,2</sup>	128.21	0	30	0.03 ± 0.01	n.d.	0.13 ± 0.09	0.13 ± 0.11	0.04	0.04	n.d.	n.d.	n.d.	1.07
nonanal <sup>1,2</sup>	142.24	0	30	0.01 ± 0.01	1.39 ± 0.49	0.12 ± 0.10	0.12 ± 0.26	0.01	0.01	n.d.	n.d.	n.d.	0.16
nopinone <sup>1</sup>	138.21	18	15	0.00 ± 0.00	0.47 ± 0.39	0.03 ± 0.02	0.03 ± 0.00	0.00	0.00	n.d.	n.d.	n.d.	1.46
camphor <sup>1</sup>	152.23	18	4.3	0.05 ± 0.00	8.86 ± 4.89	0.20 ± 0.15	0.20 ± n.d.	0.07	0.07	n.d.	n.d.	n.d.	0.02
borneol <sup>1</sup>	154.25	18	49	0.00 ± 0.00	2.31 ± 1.34	0.04 ± 0.04	0.04 ± 0.00	0.00	0.00	n.d.	n.d.	n.d.	1.78
decanal <sup>1,2</sup>	156.20	0	30	0.03 ± 0.00	3.55 ± 2.83	0.11 ± 0.09	0.11 ± 0.05	0.03	0.03	n.d.	n.d.	n.d.	1.75
undecanal <sup>1,2</sup>	170.30	0	30	0.06 ± 0.01	0.36 ± 0.14	0.01 ± 0.01	0.01 ± 0.03	0.05	0.05	n.d.	n.d.	n.d.	4.31
methylethylketone	72.11	0.6	1.2	0.05 ± 0.02	n.d.	0.02 ± 0.01	0.02 ± 0.10	0.19	0.19	n.d.	n.d.	n.d.	0.65
methylvinylketone	70.09	1	19	0.05 ± 0.02	1.36 ± 0.67	0.05 ± 0.02	0.05 ± 0.06	0.00	0.00	n.d.	n.d.	n.d.	1.07

MW = molecular weight (g mol<sup>-1</sup>); ER = emission ratio in units of ppbv per ppmv CO equivalent to mmol per mol CO, *k*OH = second-order reaction rate coefficients of VOC+ OH reaction ( $\times 10^{12}$  cm<sup>3</sup> molec<sup>-1</sup> s<sup>-1</sup>) obtained from Manion et al., (2015); SOAP = secondary organic aerosol potential values reported in Derwent et al (2010b). <sup>1</sup> denotes species whose SOAP values were estimated from the analogous species and <sup>2</sup> *k*OH values were estimated from the analogous species.

Table S2: VOC species groups based on GEIA method and mean POCP values suggested for each family (Huang et al., 2017)

Class	VOCs families	VOC species integrated in this study	Mean POCP
VOC1	Alkanols (alcohols)	n.d.	34.92
VOC2	Ethane	n.d.	12.3
VOC3	Propane	n.d.	22.12
VOC4	Butanes	n.d.	36.54
VOC5	Pentanes	pentane	39.5
VOC6	Hexanes and higher alkanes	2-methylpentane, 3-methylpentane, hexane, 2,2-dimethylpentane, 2,4-dimethylpentane, 2,2,3-trimethylbutane, 3,3-dimethylpentane, cyclohexane, 2-methylhexane, 2,3-dimethylpentane, iso-octane, heptane, octane, nonane, decane, undecane, dodecane, tridecane, tetradecane, pentadecane, hexadecane	44.15
VOC7	Ethene (ethylene)	n.d.	100
VOC8	Propene	n.d.	97.89
VOC9	Ethyne (acetylene)	n.d.	8.5
VOC10	Isoprenes	isoprene	109.2
VOC11	Monoterpenes	$\alpha$ -pinene, $\beta$ -pinene, camphene, 3-carene, $\alpha$ -terpinene, limonene, $\alpha$ -ocimene, $\gamma$ -terpinene, terpinolene, myrcene	109.2
VOC12	Other alk(adi)enes/alkynes (olefines)	n.d.	95.29
VOC13	Benzene (benzol)	benzene	21.8
VOC14	Methylbenzene (toluene)	toluene	63.7
VOC15	Dimethylbenzenes (xylenes)	m+p-xylene, o-xylene, ethylbenzene,	107.41
VOC16	Trimethylbenzenes	1,2,4-trimethylbenzene, 1,2,3-trimethylbenzene and 1,3,5-trimethylbenzene	129.86
VOC17	Other aromatics	iso-propylbenzene, styrene	77.78
VOC18	Esters	n.d.	20.68
VOC19	Ethers (alkoxy alkanes)	n.d.	12.44
VOC20	Chlorinated hydrocarbons	n.d.	23.72
VOC21	Methanal (formaldehyde)	n.d.	51.9
VOC22	Other alkanals (aldehydes)	benzaldehyde, heptanal, hexanal, octanal, nonanal, decanal, undecanal, camphor, borneol	64.1
VOC23	Alkanones (ketones)	methylvinylketone, methylethylketone	24.54
VOC24	Acids (alkanoic)	n.d.	12.44
VOC25	Other NMVOC (HCFCs, nitriles, etc.)	n.d.	12.44

POCP= photochemical ozone creation potentials (POCPs) reported on Derwent et al ( 2001, 2010)

## References

- Derwent, R. G., Jenkin, M. E., Saunders, S. M. and Pilling, M. J.: Characterization of the reactivities of volatile organic compounds using a master chemical mechanism, *J. Air Waste Manag. Assoc.*, 51(5), 699–707, doi:10.1080/10473289.2001.10464297, 2001.
- Derwent, R. G., Jenkin, M. E., Pilling, M. J., Carter, W. P. L. and Kaduwela, A.: Reactivity scales as comparative tools for chemical mechanisms., *J. Air Waste Manag. Assoc.*, 60(8), 914–924, doi:10.3155/1047-3289.60.8.914, 2010a.
- Derwent, R. G., Jenkin, M. E., Utembe, S. R., Shallcross, D. E., Murrells, T. P. and Passant, N. R.: Secondary organic aerosol formation from a large number of reactive man-made organic compounds, *Sci. Total Environ.*, 408(16), 3374–3381, doi:10.1016/j.scitotenv.2010.04.013, 2010b.
- Huang, G., Brook, R., Crippa, M., Janssens-Maenhout, G., Schieberle, C., Dore, C., Guizzardi, D., Muntean, M., Schaaf, E. and Friedrich, R.: Speciation of anthropogenic emissions of non-methane volatile organic compounds: A global gridded data set for 1970–2012, *Atmos. Chem. Phys.*, 17(12), 7683–7701, doi:10.5194/acp-17-7683-2017, 2017.
- Manion, J. A., Huie, R. E., Levin, R. D., Jr., D. R. B., Orkin, V. L., Tsang, W., McGivern, W. S., Hudgens, J. W., Knyazev, V. D., Atkinson, D. B., Chai, E., Tereza, A. M., Lin, C.-Y., Allison, T. C., Mallard, W. G., Westley, F., Herron, J. T., R. F. Hampson, A. and Frizzell, D. H.: NIST Chemical Kinetics Database, Gaithersburg, Maryland. [online] Available from: <http://kinetics.nist.gov/> (Accessed 18 April 2018), 2015.