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Supplement of

Snow scavenging and phase partitioning of nitrated and oxygenated aromatic hydrocarbons in polluted and remote environments in central Europe and the European Arctic

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Table S1. Overview of concentrations of NMAH sub-classes (ng L⁻¹) in precipitation

	NPs ^a	NCs ^b	NSAs	Total NMAHs	
Urban, western central Europe (Switzerland), rain	1659.8-3041.4 ^{TOT}	N.A.	N.A.	1659.8-3041.4 ^{TOT}	Leuenberger et al., (1988)
Urban, central Europe (Germany), rain	<300-20180 ^{TOT} (4-NP+2-NP)	N.A.	N.A.	<300-20180 ^{TOT}	Levsen et al., (1991)
Remote, central Europe (Germany), rain	6300-25700 ^{TOT} (4-NP, 3-M-4-NP, DNPs)	N.A.	N.A.	6300-25700 ^{TOT}	Herterich and Herrmann, (1990)
Urban, rural and forest, central Europe (Germany), rain	> 1000*** (4-NP), 200-800*** (other NPs)	N.A.	N.A.	N.A.	Schüssler and Nitschke (2001)
Urban background, northern Europe (Denmark), rain	1000-11900 ^{TOT} (4NP)	N.A.	N.A.	3000-18000 ^{TOT} (NPs + DNOC)	Bossi et al., (2002)
Urban background and rural, northern Europe (Denmark), rain	Rural: 4421 ^{TOT***} , Urban: 7197 ^{TOT ***} (NPs, DNPs)	N.A.	N.A.	Rural: 4421 ^{TOT***} , Urban: 7197 ^{TOT***}	Asman et al., (2005)
Urban and rural, western Europe (France), rain	Urban: 94300-102700 ^{TOT} , Rural: 71200-76800 ^{TOT}	N.A.	N.A.	Urban: 94300-102700 ^{TOT} Rural: 71200-76800 ^{TOT}	Schummer et al., (2009)
Urban, southern USA (Texas), rain	200-4890 (4-NP), 0-690 (2-NP), 40-3310 (2,4-DNP), 0-2260 (3-M-4-NP)	N.A.	N.A.	Average total: 3190	Ganranoo et al., (2010)
Urban, central Europe (Germany)	2660 – 4400 ^{TOT}	N.A.	N.A.	2660 – 4400 ^{TOT}	Alber et al., (1989)
Antarctica	5-15 ^{pa} (4-NP)	N.A.	N.A.	5-15 ^{pa} (4-NP)	Vanni et al., (2001)
Urban, central Europe (Germany, Austria, Czech Republic) 2015-17	19.5-206.2 ^{pp} 295.0-2969.2 ^{pa}	<0.56**-54.1 ^{pp} 19.5-894.9 ^{pa}	<0.56**-16.4 ^{pp} 13.0-388.4 ^{pa}	19.5-276.6 ^{pp} 291.5-4252.6 ^{pa}	This study
Rural, central Europe(Germany, Austria, Czech Republic) 2015-16	4.6-51.5 ^{pp} 553.0-1264.5 ^{pa}	<0.5**-1.7 ^{pp} 19.3-160.4 ^{pa}	<0.5*-<0.9 ^{pp**} 7.7-383.2 ^{pa}	4.6-51.5 ^{pp} 580.9-1345.3 ^{pa}	This study
Remote, European Arctic 2015	3.5 ^{pp} 361.5 ^{pa}	<0.67 ^{pp*} 3.5 ^{pa}	<1.67 ^{pp**} 22.0 ^{pa}	3.5 ^{pp} 387.0 ^{pa}	This study

^a including nitrophenols, methylnitrophenols and dinitrophenols; ^b including 4-NC, 3-M-5-NC and 4-M-5NC; ^{pp} precipitation particulate phase; ^{pa} precipitation aqueous phase; ^{TOT} total concentration in precipitation (particulate + aqueous phase); N.A.: data not available; * below limit of detection (LOD); ** below limit of quantification (LOQ); *** median concentration

Table S2. Abraham solute descriptors

Substance		E	S	A	B	V	L	Reference
1,4-Naphthoquinone	1,4-O ₂ NAP	1.08	1.13	0	0.62	1.1598	6.341	ABSOLV-EM
9-Fluorenone	9-OFLN	1.75	1.51	0	0.36	1.3722	7.568	M. Abraham
9,10-Anthraquinone	9,10-O ₂ ANT	1.41	1.7	0	0.46	1.5288	8.593	ABSOLV-EM
Benzanthrone	OBAT	2.58	1.56	0	0.49	1.7412	9.798	M. Abraham
2-Nitro-9-fluorenone	2-N-9-OFLN	2.13	2.01	0	0.48	1.5464	9.127	M. Abraham
Benzo(a)fluorenone	BaOFLN	2.58	1.82	0	0.44	1.7412	10.063	M. Abraham
Benzo(b)fluorenone	BbOFLN	2.37	1.75	0	0.67	1.7412	9.755	M. Abraham
1,2-Benzantraquinone	1,2-O ₂ BAA	2.5	2.14	0	0.6	1.8978	10.97	M. Abraham
1-Nitronaphthalene	1-NNAP	1.6	1.51	0	0.29	1.2596	7.056	M. Abraham
2-Nitronaphthalene	2-NNAP	1.6	1.5	0	0.34	1.2596	6.85	ABSOLV-EM
5-Nitroacenaphthene	5-NACE	1.86	1.56	0	0.33	1.4328	7.858	M. Abraham
2-Nitrofluorene	2-NFLU	1.85	1.7	0	0.37	1.5307	8.364	M. Abraham
9-Nitroanthracene	9-NANT	2.57	1.88	0	0.38	1.6286	9.712	M. Abraham
9-Nitrophenanthrene	9-NPHE	2.57	1.88	0	0.38	1.6286	9.712	M. Abraham
3-Nitrophenanthrene	3-NPHE	2.57	1.88	0	0.38	1.6286	9.712	M. Abraham
2-nitrofluoranthene	2-NFLT	2.87	2.09	0	0.35	1.7588	10.592	ABSOLV-CAL
3-nitrofluoranthene	3-NFLT	2.87	2.09	0	0.35	1.7588	10.592	ABSOLV-CAL
1-Nitropyrene	1-NPYR	3.07	2.15	0	0.41	1.7588	11.036	M. Abraham
2-Nitropyrene	2-NPYR	3.07	2.15	0	0.41	1.7588	11.036	M. Abraham
7-Nitrobenz(a)anthracene	7-NBAA	3.25	2.27	0	0.47	1.9976	12.21	M. Abraham
6-Nitrochrysene	6-NCHR	3.29	2.25	0	0.48	1.9976	12.23	M. Abraham
1,3-Dinitropyrene	1,3-N ₂ PYR	3.34	2.8	0	0.52	1.933	12.58	M. Abraham
1,6-Dinitropyrene	1,6-N ₂ PYR	3.34	2.8	0	0.52	1.933	12.58	M. Abraham
1,8-Dinitropyrene	1,8-N ₂ PYR	3.34	2.8	0	0.52	1.933	12.58	M. Abraham
6-Nitrobenzo(a)pyrene	6-NBAP	3.91	2.45	0	0.48	2.1278	13.62	M. Abraham
2,4-Dinitrophenol	2,4-DNP	1.2	1.49	0.09	0.56	1.1235	5.981	ABSOLV-EM
Dinitro-ortho-cresol	DNOC	1.2	1.59	0.04	0.52	1.2644	6.58	ABSOLV-EM
3-Nitrosalicylic acid	3-NSA	1.08	1.44	0.39	0.36	1.1646	6.253	ABSOLV-CAL
5-Nitrosalicylic acid	5-NSA	1.33	1.23	0.82	0.47	1.1646	6.742	ABSOLV-EM
4-Nitrophenol	4-NP	1.07	1.72	0.82	0.26	0.9493	5.876	ABSOLV-EM
4-nitroguaiacol	4-NG	1.04	1.53	0.45	0.57	1.1489	6.029	ABSOLV-CAL
3-Methyl-4-nitrophenol	3-M-4-NP	1.07	1.63	0.8	0.25	1.0902	6.06	ABSOLV-EM
2-Methyl-4-nitrophenol	2-M-4-NP	1.1	1.6	0.78	0.25	1.0902	6.324	ABSOLV-EM
4-Nitrocatechol	4-NC	1.2	1.65	1.14	0.63	1.008	6.002	ABSOLV-CAL
4-Methyl-5-nitrocatechol	4-M-5-NC	1.22	1.59	1.14	0.63	1.1489	6.474	ABSOLV-CAL
3-Methyl-5-nitrocatechol	3-M-5-NC	1.22	1.59	1.14	0.63	1.1489	6.474	ABSOLV-CAL

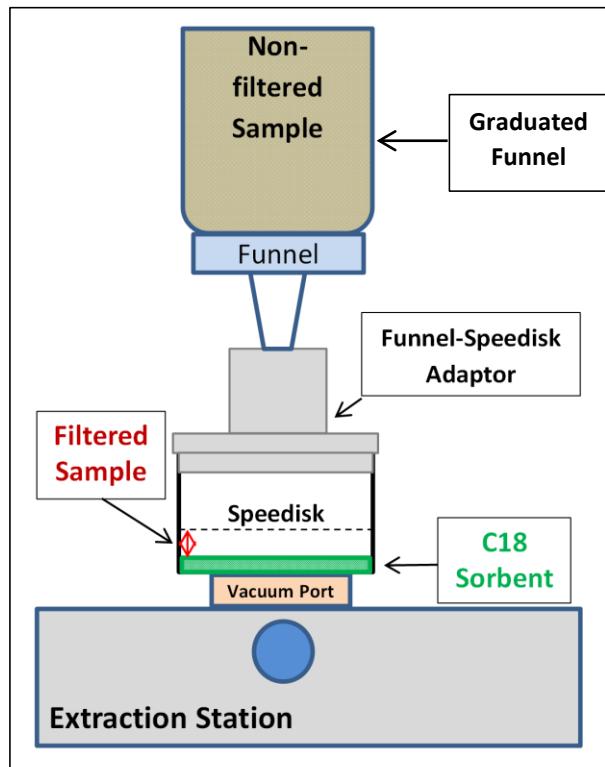
Abraham solute descriptors used in multiphase ppLFER gas-particle partitioning model. Values obtained from various sources - ABSOLV-EM (Exact Match): experimental values present in ABSOLV database; ABSOLV-CAL: values estimated by the program using substance molecular structure (ACD/Labs, 2015). The remaining values were obtained through personal communication with Michael H. Abraham, University College London.

Table S3. ppLFER system parameters for calculating K_P values and enthalpies of phase change

System	Unit	<i>e</i>	<i>s</i>	<i>a</i>	<i>b</i>	<i>v</i>	<i>l</i>	<i>c</i>	T(K)	Reference
$\log K_{\text{DMSO-air}}^{\text{a}}$	$\text{L}_{\text{air}} \text{ L}^{-1}_{\text{solvent}}$	-0.22	2.90	5.04	0.00	-	0.72	-0.56	298	Abraham et al., (2010)
$\Delta H_{\text{DMSO-air}}^{\text{b}}$	kJ mol^{-1}	-0.3	-18.4	-47.4	-5.9	-	-6.4	-2.5		Mintz et al., (2007)
$\log K_{\text{PU-air}}^{\text{c}}$	$\text{L}_{\text{air}} \text{ kg}^{-1}_{\text{PU}}$	-	1.69	3.66	0.00	0.36	0.71	-0.15	288	Kamprad and Goss, (2007)
$\Delta H_{\text{PU-air}}^{\text{d}}$	kJ mol^{-1}	-	-17.6	-46.6	-	-12.8	-4.3	2.7	-	Kamprad and Goss, (2007)
$\log K_{\text{soot-air}}^{\text{e}}$	$\text{m}^3_{\text{air}} \text{ m}^{-2}_{\text{surface}}$	-	-	2.70	2.45	-	1.09	-8.47	288	Roth et al., (2005)
$\Delta H_{\text{soot-air}}^{\text{f}}$	kJ mol^{-1}			= (-9.8 × log $K_{\text{soot-air}}$) - 90.5						Goss, (2004)
$\log K_{(\text{NH}_4)_2\text{SO}_4\text{-air}}^{\text{g}}$	$\text{m}^3_{\text{air}} \text{ m}^{-2}_{\text{surface}}$	-	-	2.13	5.34	-	0.88	-8.47	288	Goss et al., (2003)
$\log K_{\text{NaCl-air}}^{\text{h}}$	$\text{m}^3_{\text{air}} \text{ m}^{-2}_{\text{surface}}$	-	-	2.86	4.82	-	0.84	-8.47	288	Goss et al., (2003)
$\Delta H_{\text{salt-air}}^{\text{i}}$	kJ mol^{-1}			= (-10.2 × log $K_{\text{salt-air}}$) - 89.6						Goss, (2004)
$\log K_{\text{octanol-water}}^{\text{j}}$	$\text{L}_{\text{water}} \text{ L}^{-1}_{\text{octanol}}$	-	-1.41	-0.18	-3.45	2.41	0.43	0.34	298	Goss, (2005)

^{a, c} calculate logarithmic partitioning coefficients for *absorption* processes, while ^{e, g, h} calculate those for *adsorption* processes, as indicated in Eq. 4 of the main text. Enthalpies of phase change for *absorption* models ^{a, c} were calculated for each analyte using Abraham solute descriptors from Table S2 and ppLFER models ^{b, d} in Table S3, respectively. For *adsorption* models ^{e, g, h}, solute-specific enthalpies were calculated using the empirical equations ^{f, i} in Table S3 and logarithmic *adsorption* coefficients for each analyte calculated using models ^{e, g, h} at 288 K. Individual partitioning coefficients calculated for each model were un-logged and corrected for the effect of temperature at 273 K using van 't Hoff equation and the calculated enthalpies. Note that the units for these temperature-corrected partitioning coefficients must be as required in Eq. 4 of the main text, in order to calculate the final K_P ($\text{m}^3 \text{ g}^{-1}$); note the unit difference for $K_{\text{PU-air}}$ model. ^{g, h} calculate the logarithmic partitioning coefficients at 60% relative humidity.

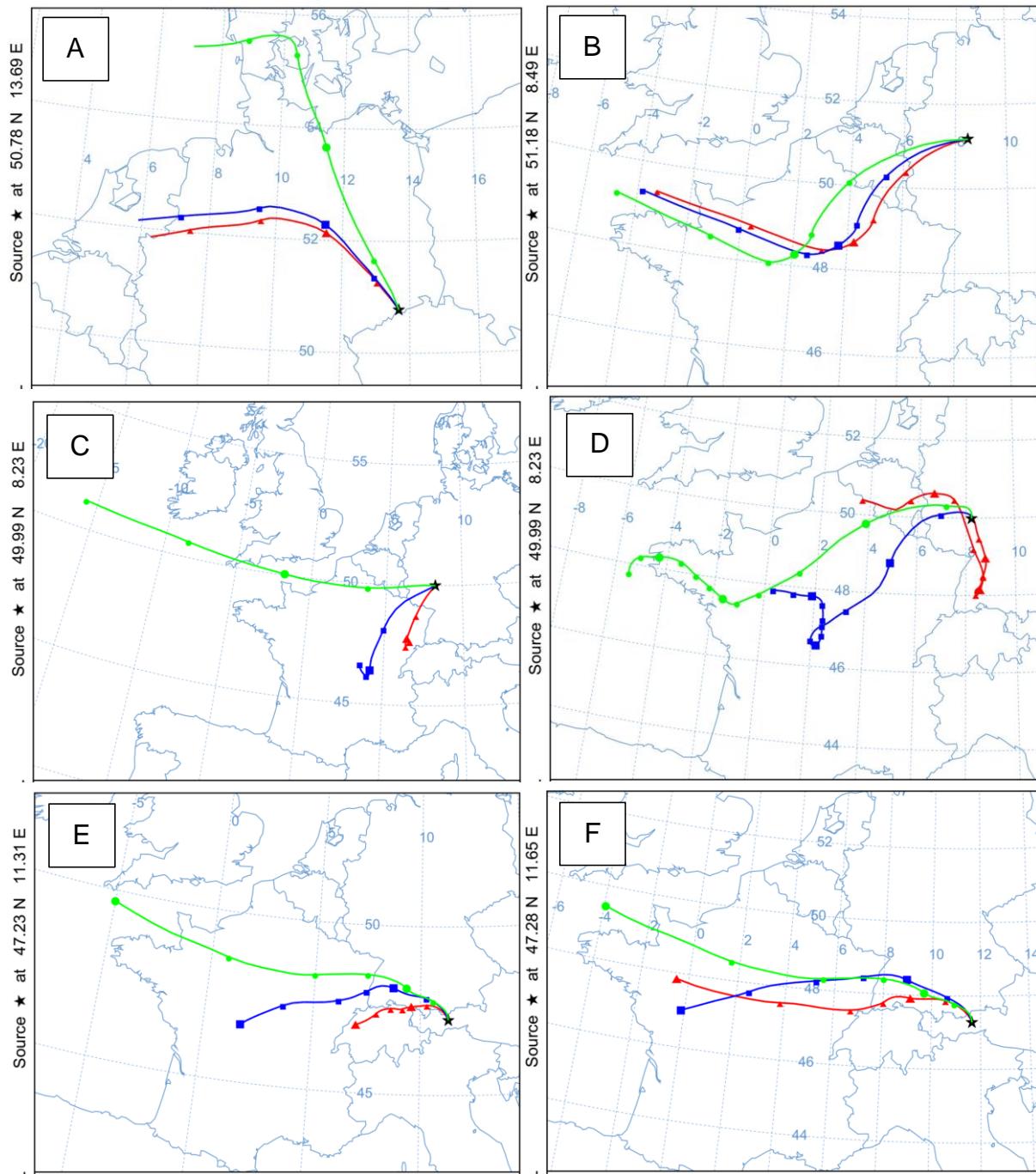
Figure S1. Snowmelt sample separation and extraction assembly



Text S1. Air mass backward trajectory analysis

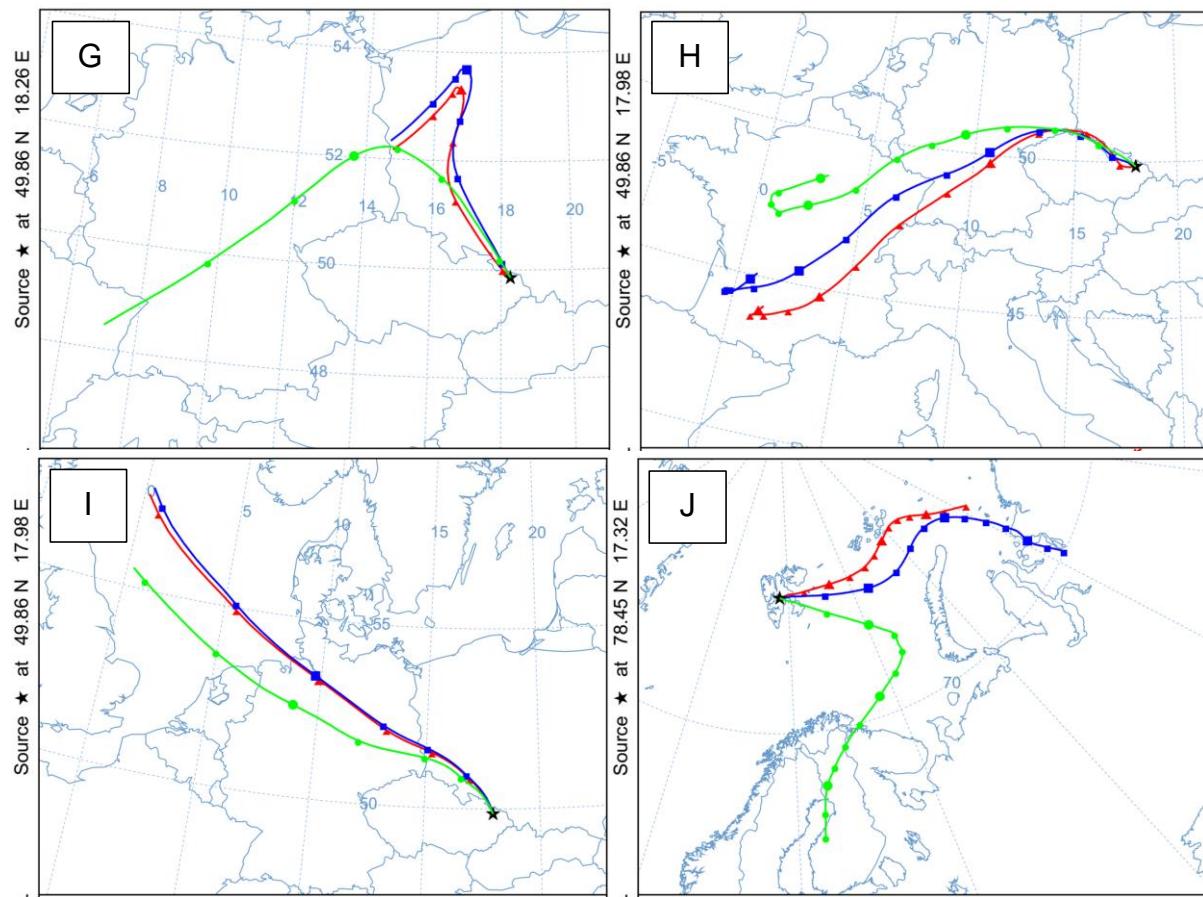
For all central European sites, the air masses corresponding to the snow samples had been advected mostly from westerly directions (Figure S2). They had passed over polluted areas of central and western Europe (such as in NE France/SW Germany, W and SE Germany for samples MZ15, OS, WB and AB) until the last 100-200 km before precipitation started, when they had been transported over rural areas. In conclusion, these air mass histories are quite typical for the region in the sense that the source areas of the region have contributed to pollution loading, while point sources or a single source area, such as a close city, was never determining the loading. The snowfalls leading to samples MZ15, OS, WB, and PP2 immediately followed frontal passages with advection from westerly directions (trajectories are shown in Figure S2), unlike in the other precipitation events. Snow fall in air masses following a frontal passage may have been on-going for some time prior to arrival. This could lead to somewhat lower concentrations in precipitation, as the gases and particles, to be eventually transferred into snow, may have been previously scavenged.

Figure S2. Air mass backward trajectories from the sites before sample collection. Tick marks indicate 6-hour intervals; colors indicate different arrival heights: red = 200, blue = 500, green = 1000 m above ground



A: Altenberg (AB), B: Winterberg (WB), C: Mainz 2015 (MZ15), D: Mainz 2017 (MZ17), E: Götzens (GS), F: Kolsassberg (KB)

Figure S2 continued



G: Ostrava (OS), H: Pustá Polom 1 (PP1), I: Pustá Polom 2 (PP2), J: Tempelfjorden (TF)

Table S4A. Total N/OPAH and NMAH concentrations in snow (dissolved + particulate; ng L⁻¹)

		MZ15 Mainz	GS Götzens	OS Ostrava	MZ17 Mainz	WB Winterberg
1,4-naphthoquinone	1,4-O ₂ NAP	<LOQ	<LOQ	17.9	7.1	<LOQ
9-fluorenone	9-OFLN	57.1	40.1	49.8	26.1	44.6
9,10-anthraquinone	9,10-O ₂ ANT	55.2	214.5	269.2	22.3	274.6
Benzanthrone	OBAT	<LOQ	<LOQ	478.3	3.3	20.1
Benz(a)fluorenone	BaOFLN	5.3	7.5	45.9	7.5	16.3
Benz(b)fluorenone	BbOFLN	2.9	8.3	36.2	6.3	18.9
1,2-Benzanthraquinone	1,2-O ₂ BAA	4.2	11.8	57.8	7.3	17.4
1-nitronaphthalene	1-NNAP	0.6	1.3	<LOQ	0.6	1.1
2-nitronaphthalene	2-NNAP	<LOQ	0.1	<LOQ	<LOQ	0.3
9-nitroanthracene	9-NANT	0.7	13.6	<LOQ	<LOQ	7.7
2-nitrofluoranthene	2-NFLT	<LOQ	2.5	11.6	2.7	0.3
2,4-dinitrophenol	2,4-DNP	17.5	23.3	73.2	32.1	125.0
Dinitro-ortho-cresol	DNOC	8.4	8.6	108.3	16.9	26.2
3-nitrosalicylic acid	3-NSA	2.7	14.3	26.4	146.0	6.0
5-nitrosalicylic acid	5-NSA	10.3	40.1	50.8	258.8	12.0
4-nitrophenol	4-NP	158.1	971.2	44.6	2262.3	760.0
4-nitroguaiacol	4-NG	<LOQ	<LOQ	155.2	325.5	<LOQ
3-methyl-4-nitrophenol	3-M-4-NP	25.7	82.1	250.6	158.3	147.7
2-methyl-4-nitrophenol	2-M-4-NP	49.3	150.5	28.4	380.2	213.9
4-nitrocatechol	4-NC	14.9	50.8	48.2	800.4	50.5
4-methyl-5-nitrocatechol	4-M-5-NC	2.4	7.1	7.7	60.2	8.0
3-methyl-5-nitrocatechol	3-M-5-NC	2.2	8.2	5.8	88.4	5.7
Σ OPAHs		124.6	282.1	955.2	79.8	391.7
Σ NPAHs		1.2	17.6	11.6	3.2	9.4
Σ NPs ^a		259.0 ^b	1235.6	660.3	3175.4	1272.8
Σ NCs		19.5 ^b	66.1	61.7	949.0	64.1
Σ NSAs		13.0 ^b	54.3	77.2	404.8	18.0

Ostrava sample was analyzed for N/OPAHs without phase separation; MZ15 sample was only analyzed for the aqueous phase; ^a Σ NPs = 4-NP + ΣM-NPs + 4-NG + 2,4-DNP + DNOC. ^b shows concentrations in the aqueous phase only because the particulate phase was not analyzed for this site due to technical issues; hence, these values were not used in stating the concentration ranges in the main text.

Table S4A continued.

		AB Altenberg	KB Kolsassberg	PP1 Pustà Polom	PP2 Pustá Polom	TF Tempelfjorden
1,4-naphthoquinone	1,4-O ₂ NAP	<LOQ	<LOQ	14.2	11.6	<LOQ
9-fluorenone	9-OFLN	38.4	55.8	37.9	53.5	2.5
9,10-anthraquinone	9,10-O ₂ ANT	258.5	335.9	222.5	595.3	<LOQ
Benzanthrone	OBAT	<LOQ	2.0	626.6	758.1	0.7
Benz(a)fluorenone	BaOFLN	16.4	27.4	78.9	95.9	0.1
Benz(b)fluorenone	BbOFLN	12.4	17.9	60.1	106.5	<LOQ
1,2-Benzanthraquinone	1,2-O ₂ BAA	17.7	23.7	86.7	136.5	0.1
1-nitronaphthalene	1-NNAP	1.0	0.5	<LOQ	<LOQ	<LOQ
2-nitronaphthalene	2-NNAP	0.2	<LOQ	<LOQ	<LOQ	<LOQ
9-nitroanthracene	9-NANT	5.0	13.2	<LOQ	<LOQ	<LOQ
2-nitrofluoranthene	2-NFLT	2.6	1.4	19.1	13.8	<LOQ
2,4-dinitrophenol	2,4-DNP	47.2	24.7	94.3	14.8	13.3
Dinitro-ortho-cresol	DNOC	14.8	6.5	85.5	12.2	3.6
3-nitrosalicylic acid	3-NSA	1.2	7.0	69.7	34.8	5.7
5-nitrosalicylic acid	5-NSA	6.6	31.2	313.5	105.5	16.3
4-nitrophenol	4-NP	566.7	564.9	18.4	15.4	310.3
4-nitroguaiacol	4-NG	18.5	<LOQ	169.4	282.3	14.8
3-methyl-4-nitrophenol	3-M-4-NP	41.3	67.5	218.6	569.1	4.6
2-methyl-4-nitrophenol	2-M-4-NP	33.9	98.8	259.3	71.9	18.4
4-nitrocatechol	4-NC	19.1	25.6	30.4	67.1	<LOQ
4-methyl-5-nitrocatechol	4-M-5-NC	6.3	4.2	2.3	61.5	<LOQ
3-methyl-5-nitrocatechol	3-M-5-NC	2.4	5.5	2.5	32.8	3.5
\sum OPAHs		343.3	462.7	1126.9	1757.4	3.5
\sum NPAHs		8.8	15.1	19.1	13.8	<LOQ
\sum NPs ^a		722.4	762.5	845.5	965.7	365.0
\sum NCs		27.7	35.3	35.2	161.4	3.5
\sum NSAs		7.7	38.2	383.2	140.4	22.0

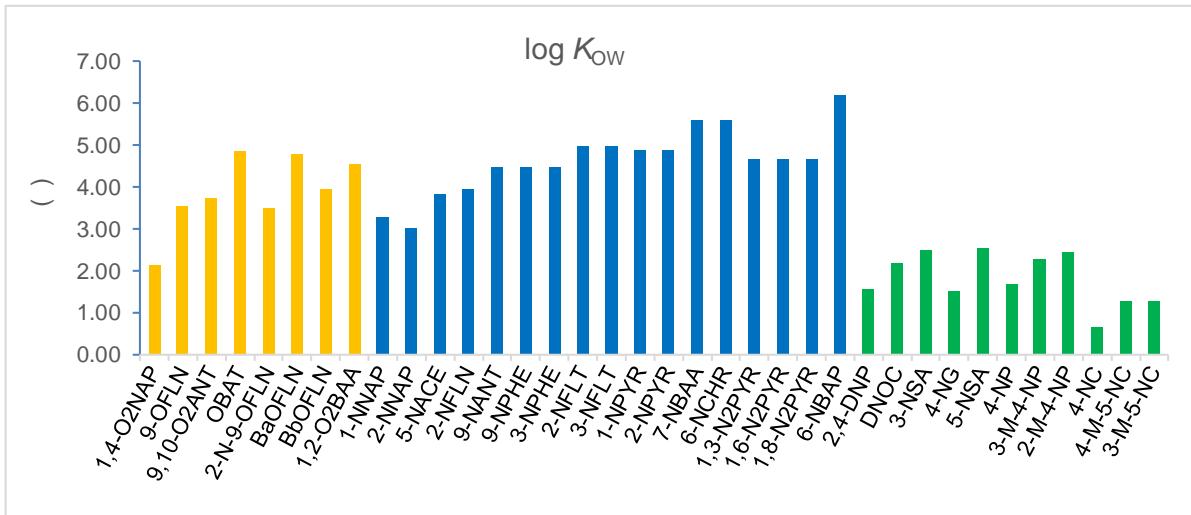
Pustà Polom samples were analyzed for N/OPAHs without phase separation; ^a \sum NPs = 4-NP + \sum M-NPs + 4-NG + 2,4-DNP + DNOC

Table S4B. Analytes in air gas and particulate phases (ng m⁻³), and in snow sample from Ostrava (OS; ng L⁻¹)

		<i>c_g</i> (ng m ⁻³)	<i>c_p</i> (ng m ⁻³)	<i>c_(pa + pp)</i> (ng l ⁻¹)	<i>W_T</i>	<i>Θ</i> 273 K	<i>log K_{ow}</i> 298 K
1,4-naphthoquinone	1,4-O ₂ NAP	0.28	0.031	18.6	6.0×10 ⁴	0.001	2.13
9-fluorenone	9-OFLN	18.9	5.0	53.9	2.3×10 ³	0.12	3.53
9,10-anthraquinone	9,10-O ₂ ANT	1.9	6.3	281.7	3.4×10 ⁴	0.81	3.74
Benzanthrone	OBAT	n.d.	12.8	478.3	3.7×10 ⁴	0.91	4.86
Benz(a)fluorenone	BaOFLN	0.16	6.5	45.9	6.9×10 ³	0.99	4.78
Benz(b)fluorenone	BbOFLN	n.d.	8.7	36.2	4.2×10 ³	0.98	3.95
1,2-benzanthraquinone	1,2-O ₂ BAA	n.d.	n.d.	57.8	n.a.		
1-nitronaphthalene	1-NNAP	0.23	0.042	n.d.	n.a.		
2-nitronaphthalene	2-NNAP	0.21	n.d.	n.d.	n.a.		
5-nitroacenaphthene	5-NACE	0.0002	0.014	n.d.	n.a.		
9-nitroanthracene	9-NANT	0.032	0.42	n.d.	n.a.		
2-nitrofluoranthene	2-NFLT	0.0010	0.55	11.6	2.1×10 ⁴	1.00	4.98
2-nitropyrene	2-NPYR	0.00013	0.16	n.d.	n.a.		
7-nitrobenz(a)anthracene	7-NBAA	n.d.	0.33	n.d.	n.a.		
6-nitrochrysene	6-NCHR	n.d.	0.031	n.d.	n.a.		
2,4-dinitrophenol	2,4-DNP	n.a.	n.d.	73.2	n.a.		
Dinitro-ortho-cresol	DNOC	n.a.	n.d.	108.3	n.a.		
3-nitrosalicylic acid	3-NSA	n.a.	0.46	26.4	5.7×10 ⁴	0.61	2.49
5-nitrosalicylic acid	5-NSA	n.a.	0.62	50.8	8.2×10 ⁴	1.00	2.54
4-nitrophenol	4-NP	n.a.	3.3	44.6	1.3×10 ⁴	1.00	1.68
4-nitroguaiacol	4-NG	n.a.	n.d.	155.2	n.a.		
3-methyl-4-nitrophenol	3-M-4-NP	n.a.	1.6	250.6	1.6×10 ⁵	1.00	2.27
2-methyl-4-nitrophenol	2-M-4-NP	n.a.	2.1	28.4	1.3×10 ⁴	1.00	2.43
4-nitrocatechol	4-NC	n.a.	17.3	48.2	2.8×10 ³	1.00	0.64
4-methyl-5-nitrocatechol	4-M-5-NC	n.a.	7.1	7.7	1.1×10 ³	1.00	1.27
3-methyl-5-nitrocatechol	3-M-5-NC	n.a.	5.3	5.8	1.1×10 ³	1.00	1.27

c_g: analyte concentrations in the gas phase, *c_p*: concentrations in the particulate phase, *c_(pa + pp)*: sum of the concentrations in snow aqueous and particulate phases; *W_T*: total scavenging ratio (dimensionless) = [*c_(pa + pp)* (ng L⁻¹) × 1000]/ [*c_g* + *c_p* (ng m⁻³)]; *W_T* was only determined for substances that were detected in both air and snow samples; n.d.: not detected; n.a.: not available; *Θ*: particulate mass fraction = *c_p* / (*c_g* + *c_p*); the table only lists substances which were detected in either air or snow samples. NMAH concentrations were not determined in the gas phase; however, except for 2,4-dinitrophenol and dinitro-ortho-cresol, which were not found in the air particulate phase, based on our modeled particulate mass fractions (Figure 6C), we expect the rest of NMAHs to be mainly in the particulate phase at near zero temperatures. Therefore, we do not expect the lack of NMAH measurement in the gas phase to have any significant effect on the calculated *W_T* values.

Figure S3 Octanol-water partitioning coefficient, $\log K_{\text{ow}}$, calculated using ppLFER model in Table S3



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