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Dataset name: **iCUPE Dataset (DS) from Deliverable 2.4.1:**

DS on emerging organic contaminants in air from the Arctic

Author(s) and affiliations: **Dr. Zhiyong Xie**

HZG - Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research GmbH

Place and date: **Geesthacht, Germany, 31 Dec 2018**

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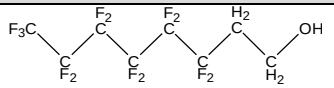
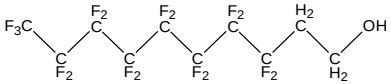
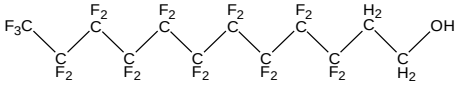
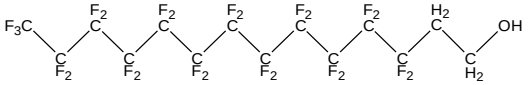
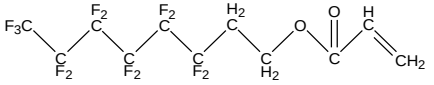
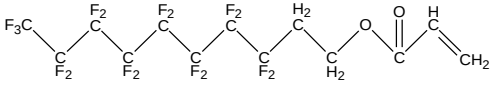
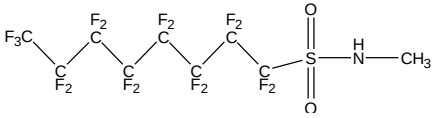
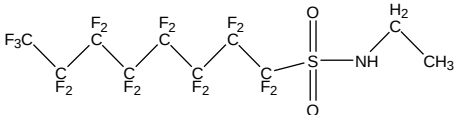
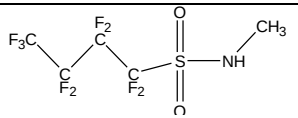
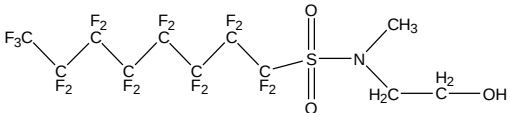
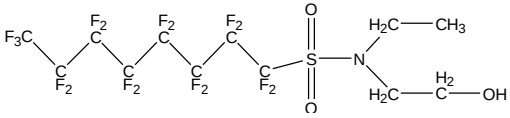
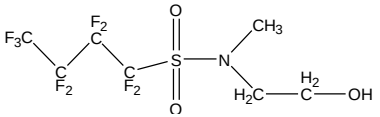
The produced dataset (in MS Excel format) contains concentrations of neutral PFASs in vapor and particle phases of air samples (in total 44) collected at Ny-Alesund (Norway) (78.917° N, 11.933° E) from 27th September 2011 until 29th August 2012. The concentrations for 12 different PFASs are given in pg/m^3. For each of 12 PFASs, the values for average blank (n=10), standard deviation, and method detection limit (MDL) are included. As 8:2 FTA, EtFOSA, MeFBSA and MeFBSE are not detectable in all filter blanks, their MDLs are set as 0 for particle phase in this work. In addition, an annex (Table) contains information on full names, acronyms, Chemical Abstract System (CAS) numbers, molecular weight (MW), chemical structure, method detection limits (MDL) and compound descriptors of the 12 PFASs.

Table 1. Full names, acronyms, Chemical Abstract System (CAS) numbers, molecular weight (MW), structure, method detection limits (MDL) and compound descriptors of the 12 PFASs

Full name	CAS number	Abbr.	MW (g/mol)	Structure
6:2 Fluorotelomer alcohol	647-42-7	6:2 FTOH	364.1	
8:2 Fluorotelomer alcohol	678-39-7	8:2 FTOH	464.1	
10:2 Fluorotelomer alcohol	865-86-1	10:2 FTOH	564.1	
12:2 Fluorotelomer alcohol	39239-77-5	12:2 FTOH	664.2	
6:2 Fluorotelomer acrylate	17527-29-6	6:2 FTA	418.2	
8:2 Fluorotelomer acrylate	27905-45-9	8:2 FTA	518.2	
N-methyl perfluorooctane sulfonamide	31506-32-8	MeFOSA	513.2	
N-ethyl perfluorooctane sulfonamide	4151-50-2	EtFOSA	527.2	

N-methyl perfluorobutane sulfonamide	68298-12-4	MeFBSA	313.1	
N-methyl perfluorooctane sulfonamidoethanol	24448-09-7	MeFOSE	557.2	
N-ethyl perfluorooctane sulfonamidoethanol	1691-99-2	EtFOSE	571.3	
N-methyl perfluorobutane sulfonamidoethanol	34454-97-2	MeFBSE	357.2	

Dataset name: **iCUPE Dataset (DS) Deliverable 2.4.1:**

DS on emerging organic contaminants in snow from the Arctic

Author(s) and affiliations: **Dr. Zhiyong Xie**

HZG - Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research GmbH

Place and date: **Geesthacht, Germany, 31 May 2019**

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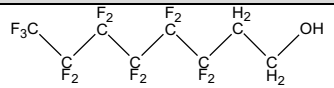
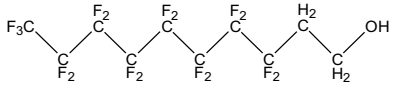
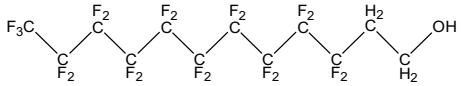
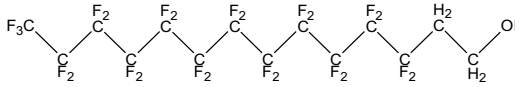
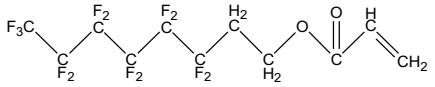
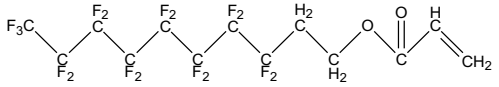
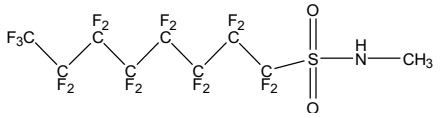
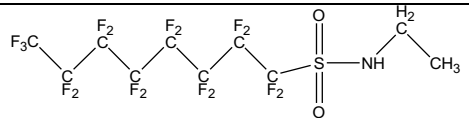
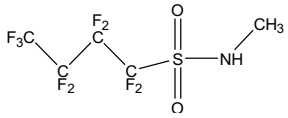
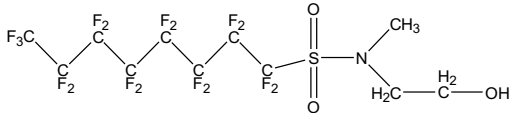
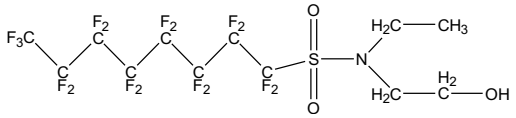
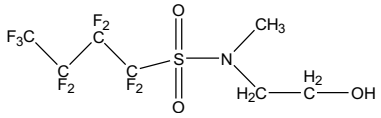
The produced dataset (in MS Excel format) contains concentrations of neutral PFASs in snow samples (in total 9) collected at Ny-Alesund (Norway) (78.917° N 11.933° E) from January to May 2012. The concentrations for 12 different PFASs are given in pg/L. For each of 12 PFASs, the values for average blank (n=5), standard deviation, and method detection limit (MDL) are included. In addition, an annex (Table) contains information on full names, acronyms, Chemical Abstract System (CAS) numbers, molecular weight (MW), chemical structure, compound descriptors of the 12 PFASs

Table 1. Full names, acronyms, Chemical Abstract System (CAS) numbers, molecular weight (MW), structure, method detection limits (MDL) and compound descriptors of the 12 PFASs

Full name	CAS number	Abbr.	MW (g/mol)	Structure
6:2 Fluorotelomer alcohol	647-42-7	6:2 FTOH	364.1	
8:2 Fluorotelomer alcohol	678-39-7	8:2 FTOH	464.1	
10:2 Fluorotelomer alcohol	865-86-1	10:2 FTOH	564.1	
12:2 Fluorotelomer alcohol	39239-77-5	12:2 FTOH	664.2	
6:2 Fluorotelomer acrylate	17527-29-6	6:2 FTA	418.2	
8:2 Fluorotelomer acrylate	27905-45-9	8:2 FTA	518.2	
N-methyl perfluorooctane sulfonamide	31506-32-8	MeFOSA	513.2	

N-ethyl perfluorooctane sulfonamide	4151-50-2	EtFOSA	527.2	
N-methyl perfluorobutane sulfonamide	68298-12-4	MeFBSA	313.1	
N-methyl perfluorooctane sulfonamidoethanol	24448-09-7	MeFOSE	557.2	
N-ethyl perfluorooctane sulfonamidoethanol	1691-99-2	EtFOSE	571.3	
N-methyl perfluorobutane sulfonamidoethanol	34454-97-2	MeFBSE	357.2	

Dataset name: **iCUPE Dataset (DS) from Deliverable 2.4.1:**

DS on emerging organic contaminants in seawater from the Arctic

Author(s) and affiliations: **Dr. Zhiyong Xie**

HZG - Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research GmbH

Place and date: **Geesthacht, Germany, 23 September 2019**

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The produced dataset (in MS Excel format) contains concentrations of organophosphate esters (OPE) in surface seawater samples (in total 22) collected in European Arctic during an expedition with R/V Polarstern from 5th June to 3rd July 2014. The spatial distribution of seawater samples is shown in Figure 1. The concentrations for 8 different OPEs are given in pg/L. For each of 8 OPEs, the values for average blank (n=4), standard deviation, and method detection limit (MDL) are included. In addition, an annex (Table 1) contains information on full names, acronyms, Chemical Abstract System (CAS) numbers, molecular weight (MW), and compound descriptors of the 8 OPEs.

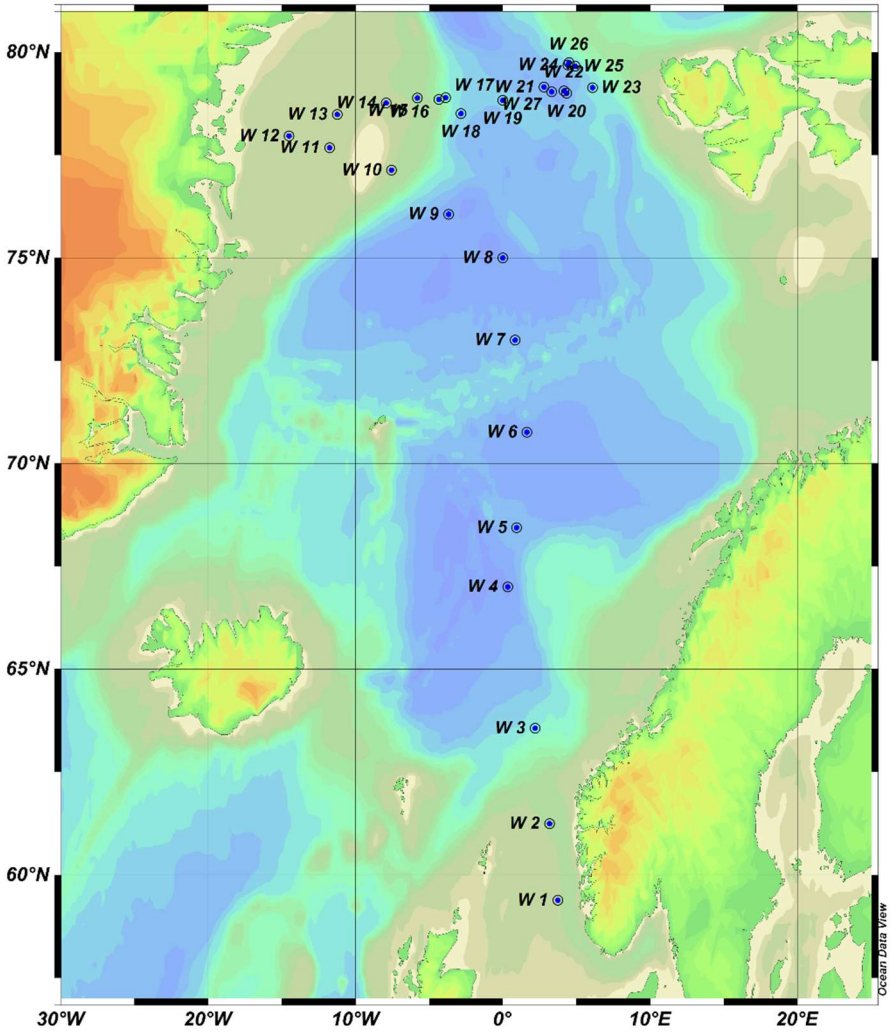

Figure 1. Sampling positions of 1-L seawater samples during *R/V Polarstern* cruise (PS85) from 5th June to 3rd July 2014.

Table 1. Full names, acronyms, Chemical Abstract System (CAS) numbers, molecular weight (MW) of the 8 organophosphate esters (OPEs).

Name	Akronym	CAS No.	Chemical form	MW
Tris-(1-chloro-2-propyl) phosphate	TCPP	13674-84-5	$C_9H_{18}Cl_3O_4P$	327.6
Tris-(2-chloroethyl) phosphate	TCEP	115-96-8	$C_6H_{12}Cl_3O_4P$	285.5
Tri-(dichlorisopropyl) phosphate	TDCPP	13674-87-8	$C_9H_{15}Cl_6O_4P$	430.9
Tri-iso-butyl phosphate	TiBP	126-71-6	$C_{12}H_{27}O_4P$	266.3
Tri-n-butyl phosphate	TBP	126-73-8	$C_{12}H_{27}O_4P$	266.3
Tripentyl phosphate	TPeP	2528-38-3	$C_{15}H_{33}O_4P$	308.4
Triphenyl phosphate	TPhP	115-86-6	$C_{18}H_{15}O_4P$	326.3
Tris-(2-ethylhexyl) phosphate	TEHP	78-42-2	$C_{24}H_{51}O_4P$	434.6