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Fact Cards of Major Groups of Per- and Polyfluoroalkyl Substances (PFASs)

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Fact Cards of Major Groups of Per- and Polyfluoroalkyl Substances (PFASs)



A cooperative agreement among FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD

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FACT CARDS OF MAJOR GROUPS OF PER- AND POLYFLUOROALKYL SUBSTANCES (PFASS)

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Table of contents

Background, aims and scope
1. Perfluoroalkyl phosphonic (a) and phosphinic acids (b) (PFPAs & PFPIAs) 10
2. Perfluoroalkyl carboxylic (a) and dicarboxylic (b) acids
3. Perfluoroalkane sulfonic (a) and sulfinic (b) acids
4. Per- and polyfluoroalkylether carboxylic (a) and sulfonic (b) acids 42
5. Perfluoroalkanoyl fluorides (a) and their derivatives (b)
6. Perfluoroalkanesulfonyl fluorides (a) and their derivatives (b)
7. n:2 Fluorotelomer-based compounds 58
8. n:1 Fluorotelomer-based compounds
9. Perfluoroalkylethers (a), epoxides (b), and vinyl ethers (c) (non-polymers)
10. Perfluoroalkenes (a) and derivatives (b)
11. Specific hydrofluoro-carbons (a), -ethers (b), and -olefins (c)
12. Side-chain fluorinated aromatics 79
13. Fluoropolymers
14. Fluoroelastomers
15. Perfluoropolyethers
Annex A. List of PFASs Included in the Fact Cards, Their Acronyms, CAS Registry Numbers (CASRNs), DTXSIDs and Fact Card Location

Background, aims and scope

The OECD/UNEP Global PFC Group¹ was established to respond to the Resolution II/5 adopted at the second session of the UN International Conference on Chemicals Management (ICCM 2) in 2009, which calls upon intergovernmental organizations, governments and other stakeholders to "consider the development, facilitation and promotion in an open, transparent and inclusive manner of national and international stewardship programmes and regulatory approaches to reduce emissions and the content of relevant perfluorinated chemicals of concern in products and to work toward global elimination, where appropriate and technically feasible". Further work on this resolution was reaffirmed in Resolution III/3 adopted at ICCM 3 noting that a significant need remains for additional work to support implementation of Resolution II/5. This report is prepared within the framework of the Group. For more details on the Group and its work, see the OECD PFAS web portal (https://oe.cd/2M9).

This document contains a set of 15 fact cards² on major groups of per- and polyfluoroalkyl substances (PFASs), prepared by the OECD/UNEP Global PFC Group between June 2018 and June 2021. The fact cards aim to provide non-expert stakeholders a quick initial glance into these groups of PFASs with some basic information on: (1) chemical identities³, synthesis and inherent properties such as bioaccumulation and transformation, (2) historical and ongoing industrial practices and commercial uses of some major commercial products, (3) regulatory status, (4) examples of reported occurrences in the environment and humans, and (5) major knowledge gaps in terms of previous sections. The fact cards also provide references where interested readers may find additional information; note that due to the fast-moving nature of the science and knowledge on PFASs, the listed references are by no means complete. For information and practical guidance on the use of terminology in regard to PFASs, readers are referred to the OECD PFAS Terminology report⁴.

It should also be noted that health and environmental effects of PFASs are not included in the fact cards. For a number of well-studied legacy PFASs, most notably perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS), a wealth of knowledge on their related environmental and human health effects have been studied and synthesized, demonstrating that they may cause a wide range of adverse health effects. These studies have played a key role in the decision making of existing regulatory actions on them, including restrictions and setting up health guideline values. For many other PFASs, considerable efforts are being made to study their health and environmental effects; existing evidence shows that exposure to many novel and emerging PFASs may result in adverse

¹ The term "PFC" in "OECD/UNEP Global PFC Group" refers to "per- and polyfluorinated chemicals", and not to perfluorocarbons. "Per- and polyfluorinated chemicals" or "PFCs" were widely used before the more precise term "per- and polyfluoroalkyl substances" was recommended by Buck et al. in 2011. As it is part of the official name of the Group, it remains unchanged here.

² Note that one fact card may contain more than one groups of PFASs that may share some similarities, e.g. in terms of structural traits, characteristics or uses; however, this arrangement does not imply any grouping strategies for PFASs.

³ Note that the Markush structure representations and molecular formulas in each fact card represent only the linear isomer of the respective substances. In reality, for many PFASs, branched or cyclic isomers have also been generated, and may be identified in products or the environment.

⁴ OECD (2021), Reconciling Terminology of the Universe of Per- and Polyfluoroalkyl Substances: Recommendations and Practical Guidance, OECD Series on Risk Management, No. 61, OECD Publishing, Paris, <u>https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/terminology-per-and-polyfluoroalkyl-substances.pdf</u>.

health and environmental effects of concern, including similar adverse effects as the PFASs that they replace (though possibly with different mechanisms of action). Interested readers are strongly recommended to consult the following sources, references therein, and other sources for information on the health and environmental effects of PFASs:

- DeWitt JC (ed.), 2015. *Toxicological effects of perfluoroalkyl and polyfluoroalkyl substances*. Springer International Publishing, Switzerland. https://doi.org/10.1007/978-3-319-15518-0.
- National Toxicology Program, 2016. Monograph on immunotoxicity associated with exposure to perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) https://ntp.niehs.nih.gov/ntp/ohat/pfoa pfos/pfoa pfosmonograph 508.pdf.
- International Agency for Research on Cancer (IARC), 2017. *Some chemicals used as solvents and in polymer manufacture*. IARC Monographs on the Evaluation of Carcinogenic Risks to Human, Volume 110. <u>https://publications.iarc.fr/547</u>.
- Pelch KE, Reade A, Wolffe TAM, Kwiatkowski CF. 2019. PFAS health effects database: Protocol for a systematic evidence map. *Environment International* 130, 104851, <u>https://doi.org/10.1016/j.envint.2019.05.045</u>; <u>https://pfastoxdatabase.org</u>.
- Ankley GT, Cureton P, Hoke RA, Houde M, Kumar A, Kurias J, Lanno R, McCarthy C, Newsted J, Salic CJ, Sample BE, Sepúlveda MS, Steevens J, Valsecchi S. 2020. Assessing the ecological risks of per- and polyfluoroalkyl substances: current state-of-the science and a proposed path forward. Environmental Toxicology and Chemistry 40(3), 564–605. https://doi.org/10.1002/etc.4869.
- Fenton SE, Ducatman A, Boobis A, DeWitt JC, Lau C, Ng C, Smith JS, Roberts SM. 2020. Per- and polyfluoroalkyl substance toxicity and human health review: Current state of knowledge and strategies for informing future research. *Environmental Toxicology and Chemistry*, 40(3), 606–630. https://doi.org/10.1002/etc.4890.
- Interstate Technology Regulatory Council (ITRC), 2020. *PFAS Fact Sheets* 7. *Human and Ecological Health Effects of select PFAS*. <u>https://pfas-1.itrcweb.org/7-human-and-ecological-health-effects-of-select-pfas/</u>.
- Lohmann R, Cousins IT, DeWitt JC, Glüge J, Goldenman G, Herzke D, Lindstrom AB, Miller MF, Ng CA, Patton S, Scheringer M, Trier X, Wang Z. 2020. Are fluoropolymers really of low concern for human and environmental health and separate from other PFAS? *Environmental Science & Technology* 54(20), 12820– 12828. <u>https://doi.org/10.1021/acs.est.0c03244</u>.
- Hodnebrog Ø, Aamaas B, Fuglestvedt JS, Marston G, Myhre G, Nielsen CJ, Sandstad M, Shine KP, Wallington TJ. 2020. Updated global warming potentials and radiative efficiencies of halocarbons and other weak atmospheric absorbers. *Reviews of Geophysics* 58, e2019RG000691. https://doi.org/10.1029/2019RG000691.
- Agency for Toxic Substances and Disease Registry (ATSDR). 2021. Toxicological profile for Perfluoroalkyls. United States Department of Health and Human Services, Public Health Service. https://wwwn.cdc.gov/TSP/ToxProfiles/ToxProfiles.aspx?id=1117&tid=237; p C8 Science Panel. C8 Study Publications. http://www.c8sciencepanel.org/publications.html.

1. Perfluoroalkyl phosphonic (a) and phosphinic acids (b) (PFPAs & PFPIAs)

Key publication: Wang, Z., Cousins, I. T., Berger, U., Hungerbühler, K. & Scheringer, M. Comparative assessment of the environmental hazards of and exposure to perfluoroalkyl phosphonic and phosphinic acids (PFPAs and PFPIAs): Current knowledge, gaps, challenges and research needs. *Environ. Int.* 89–90, 235–247 (2016).

Chemical Infor	Chemical Information & Properties					
Identification an	Identification and Terminology					
Name	Perfluoroalkyl phosphonic acids	Perfluoroalkyl phosphinic acids				
Other Names	Phosphonic acid, perfluoro-alkyl derivatives[1]; perfluoroalkyl phosphonic acids [1]; mono-substituted perfluorinated phosphonic acids [2]	Phosphinic acid, bis(perfluoro-alkyl) derivatives [1]; bis(perfluoroalkyl) phosphinic acids [1]; di-substituted perfluorinated phosphonic acids [2]				
Acronym	PFPAs	PFPIAs				
Chemical Formula	$C_n F_{2n+1} P(=O)(OH)_2$ e.g. $4 \le n \le 12$	$\begin{array}{l} C_{n}F_{2n+1}P(=\!O)(OH)(C_{m}F_{2m+1}) \\ \mbox{e.g. } 4 \leq n, m \leq 12 \end{array}$				
General Structure (only linear isomers shown here)	F = OH $F = C = P = OH$ $F = OH$ $F = OH$	$ \begin{array}{c c} F & OH & F \\ \hline F & \hline \\ F & \hline \\ \hline \\ F & \hline \\ F & O & F \end{array} $				
US EPA CompTox Markush ID	DTXSID801024679	DTXSID101024680				
Common Terminology	e.g. perfluorooctyl phosphonic acid (C ₈ PFPA)	e.g. bis(perfluorooctyl) phosphinic acid (C ₈ /C ₈ PFPIA)				
Degradability, N	Aobility, Bioconcentration					
Abiotic degradation	No degradation when exposed to heat, oxidants, and bases [3]	Hydrolyzes to yield PFPAs and $C_nF_{2n+1}H$ (a PFCA precursor) when exposed to heat or bases [3]				
Biodegradation	No aerobic biodegradation in surface water [3]	Biotransforms to yield PFPAs in rainbow trout [3]				
Adsorption on organic matter (log K _d , cm ³ /g)	C ₆ PFPA: -0.15 (soil) C ₈ PFPA: 0.89 (soil), 1.07 (sludge) C ₁₀ PFPA: 1.1 (soil), 1.17–1.63 (sludge) [3]	C ₆ /C ₆ PFPIA: 1.70 (soil) C ₆ /C ₈ PFPIA: 2.09 (soil) C ₈ /C ₈ PFPIA: 1.96 (soil) [3]				
Sorption in soils	C ₆ PFPA: 90% remaining in aqueous phase after 24 h; C ₈ PFPA: 60% remaining in aqueous phase after 24 h; C ₁₀ PFPA: 15% remaining in aqueous phase after 24 h; [4]	C ₆ /C ₆ PFPIA: 10% remaining in aqueous phase after 24 h; C ₆ /C ₈ PFPIA, C ₈ /C ₈ -PFPIA: <lod remaining<br="">in aqueous phase after 24 h; [4]</lod>				

on potentialElimination in rainbow trout [5]: t_{12} (Ce $PFPA$) = 4.4 d t_{12} (Ce $PFPA$) = 5.3 d t_{12} (Ce $PFPA$) = 5.4 d d t_{12} (Ce $PFPA$) = 5.3 d t_{12} (Ce $PFPA$) = 5.3 d t_{12} (Ce $PFPA$) = 5.4 d d t_{12} (Ce $PFPA$) = 5.7 d d t_{12} (Ce $PFPA$) = 5.2 d d d , 5.2.1 (2) t_{12} (Ce $PFPA$) = 5.2 d d d , 5.2.3 (2) t_{12} (Ce $PFPA$) = 5.2.1 d d , 5.2.3 (2) $exposed to mixture of PFAs; fish were exposed to mixture of PFPAs; fish were exposed to mixture o$	Bioaccumulati	Binds to proteins and blood cells [3]	Binds to proteins [3]
Image: transmission of the second state state state state second stat	on potential	Elimination in rainbow trout [5]:	Elimination in rainbow trout [5]:
		$t_{1/2} (C_6 PFPA) = 0.13 d$	$t_{1/2} (C_6/C_6 PFPIA) = 5.5 d$
Image: base of the state of		$t_{1/2}$ (C ₈ PFPA) = 4.4 d	$t_{1/2}$ (C ₆ /C ₈ PFPIA) = 20.4 d
Elimination in rats [2]: $t_{12}(C_6 PFPA) = 0.96 d(3), \leq 1.6 (?)$ $t_{12}(C_6 PFPA) = 1.6 d(3), \leq 2.1 (?)$ $t_{12}(C_6 C_6 PFPIA) = 1.6 d(3)$ $t_{12}(C_6 C_6 PFPIA) $		$t_{1/2} (C_{10} PFPA) = 5.3 d$	$t_{1/2}$ (C ₈ /C ₈ PFPIA) = 52.7 d
		Elimination in rats [2]:	Elimination in rats [2]:
$ \begin{array}{llllllllllllllllllllllllllllllllllll$		$t_{1/2} (C_6 PFPA) = \le 0.96 d (\circlearrowright), \le 1.6 (\circlearrowright)$	$t_{1/2}$ (C ₆ /C ₆ PFPIA) = ≤ 1.8 d (\circ), ≤ 2.3 (\circ)
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		$t_{1/2}$ (C ₈ PFPA) = ≤1.6 d (♂), ≤2.1 (♀)	$t_{1/2} (C_6/C_8 \text{ PFPIA}) = \le 2.0 \text{ d} (\bigcirc), \le 2.7 (\bigcirc)$
Image: transmission of the second state of the se		$t_{1/2} (C_{10} \text{ PFPA}) = \leq 2.5 \text{ d} (\bigcirc), \leq 2.8 (\bigcirc)$	$t_{1/2}$ (C ₈ /C ₈ PFPIA) = $\leq 2.7 \text{ d}$ (\bigcirc), ≤ 4.0 (\bigcirc)
LineL			$t_{1/2} (C_6/C_{10} \text{ PFPIA}) = \le 2.0 \text{ d} (\bigcirc), \le 3.0 (\bigcirc)$
Indication $I_{1/2} (C_v C_{12} PFPIA) = \leq 5.4 d(3), \leq 8.4 (Q)$ BCF weaky state (2ebrafish, whole body)15.8–200 L/kg [6] (for $C_h C_h S_h$ and $C_{10} PFPAs; fish wereexposure levels)3.9x10-1.58×100 L/kg [6](for C_v C_h C_h C_h C_h C_h C_h C_h C_h C_h C_h$			$t_{1/2} (C_8/C_{10} \text{ PFPIA}) = \le 5.1 \text{ d} (\bigcirc), \le 9.3 (\bigcirc)$
BCF_steady state (zebrafish, whole body)15.8–200 L/kg [6] (for C, C, a, cand Cn PFPAs; fish were exposed to mixture of PFAs at two different exposure levels) $3.9\times10^4-1.58\times10^9 L/kg [6]$ (for C/C, C, C/C, K, C, C/C, a, C/C, C/C			$t_{1/2} (C_6/C_{12} \text{ PFPIA}) = \le 5.4 \text{ d} (3), \le 8.4 (3)$
(zebrafish, whole body)(for $C_6, C_8, and C_{10}$ PFPAs; fish were exposed to mixture of PFAS at two different exposure levels)(for $C_6/C_8, C_8/C_8, C_$	BCF steady state	15.8–200 L/kg [6]	3.9×10 ⁴ -1.58×10 ⁹ L/kg [6]
While body?exposed to mixture of PFAS at two different exposure levels? C_r/C_{12} PFPIAs; fish were exposed to mixture of PFAS at two different exposure levels?SynthesisStarting material: perfluoroalkyl iodides (PFAIs, often as a mixture of linear homologs) $6 C_n F_{2n+1} I + P_4 \stackrel{heat}{\longrightarrow} 2 C_n F_{2n+1} PI_2 + 2 (C_n F_{2n+1})_2 PI$ Then, either $C_n F_{2n+1} PI_2$ or $(C_n F_{2n+1})_2 PI + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PO(OH)_2$ or $(C_n F_{2n+1})_2 PO(OH)$ or $C_n F_{2n+1} PI_2$ or $(C_n F_{2n+1})_2 PI + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PO(OH)_2$ or $(C_n F_{2n+1})_2 PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Maine Masurf-780 [2]Masurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: 10% C_6 PFPA, 8% C_8 PFPA, 5% C_{10} PFPA 37% C_6/C_6 PFPIA, 33% C_6/C_8 PFPIA, 27% C_8/C_8 PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number5229-25-9CompositionC_4/C_4-PFIA [3], [8]	(zebrafish,	(for C_6 , C_8 , and C_{10} PFPAs; fish were	(for C_6/C_6 , C_6/C_8 , C_8/C_8 , C_6/C_{10} , C_8/C_{10} , and
SynthesisMain Synthesis Method [3]Starting material: perfluoroalkyl iodides (PFAIs, often as a mixture of linear homologs) $6 C_n F_{2n+1} l + P_4 \stackrel{heat}{\longrightarrow} 2 C_n F_{2n+1} Pl_2 + 2 (C_n F_{2n+1})_2 Pl$ Then, either $C_n F_{2n+1} Pl_2 \text{ or } (C_n F_{2n+1})_2 Pl + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PO(OH)_2 \text{ or } (C_n F_{2n+1})_2 PO(OH)$ or $C_n F_{2n+1} Pl_2 \text{ or } (C_n F_{2n+1})_2 Pl + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PO(OH)_2 \text{ or } (C_n F_{2n+1})_2 PO(OH)$ Atternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]MaineMasurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: 10% C_6 PFPA, 8% C_8 PFPA, 5% C_{10} PFPA 37% C_6/C_6 PFPIA, 33% C_6/C_8 PFPIA, 27% C_8/C_8 PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number52299-25-9CompositionC_4/C_4-PFPIA [3], [8]	whole body)	exposed to mixture of PFAS at two different	C_6/C_{12} PFPIAs; fish were exposed to mixture of PEAS at two different exposure levels)
SynthesisMain Synthesis Method [3]Starting material: perfluoroalkyl iodides (PFAIs, often as a mixture of linear homologs) $6 C_n F_{2n+1} I + P_4 \stackrel{heat}{\longrightarrow} 2 C_n F_{2n+1} PI_2 + 2 (C_n F_{2n+1})_2 PI$ Then, either 		exposure levels)	of FTAS at two allferent exposure levels)
Main Synthesis Method [3]Starting material: perfluoroalkyl iodides (PFAIs, often as a mixture of linear homologs) $6 C_n F_{2n+1}I + P_4 \stackrel{heat}{\longrightarrow} 2 C_n F_{2n+1}PI_2 + 2 (C_n F_{2n+1})_2 PI$ Then, either $C_n F_{2n+1}PI_2$ or $(C_n F_{2n+1})_2 PI + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1}PO(OH)_2$ or $(C_n F_{2n+1})_2 PO(OH)$ or $C_n F_{2n+1}PI_2$ or $(C_n F_{2n+1})_2 PI + AgCl \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1}PCl_2$ or $(C_n F_{2n+1})_2 PCl$ $C_n F_{2n+1}PCl_2$ or $(C_n F_{2n+1})_2 PCl + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1}PO(OH)_2$ or $(C_n F_{2n+1})_2 PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably $n = 2$ or $n = 4$. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Maior Commercial UsesMasurf-780 [2]MameMasurf-780 [2]Name80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: $10\% C_6 PFPA, 8\% C_8 PFPA, 5\% C_{10} PFPA37\% C_6/C_6 PFPIA, 33\% C_6/C_8 PFPIA, 27\% C_8/C_8 PFPIA(amounting to 120\%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number52299-25-9CompositionC_4/C_4-PFPIA [3], [8]$	Synthesis		
Method [3] $6 C_n F_{2n+1}I + P_4 \stackrel{heat}{\longrightarrow} 2 C_n F_{2n+1}PI_2 + 2 (C_n F_{2n+1})_2 PI$ Then, either $C_n F_{2n+1}PI_2 \text{ or } (C_n F_{2n+1})_2 PI + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PO(OH)_2 \text{ or } (C_n F_{2n+1})_2 PO(OH)$ or $C_n F_{2n+1}PI_2 \text{ or } (C_n F_{2n+1})_2 PI + AgCl \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PCl_2 \text{ or } (C_n F_{2n+1})_2 PCl$ $C_n F_{2n+1}PCl_2 \text{ or } (C_n F_{2n+1})_2 PCl + H_2 O \stackrel{oxidant}{\longrightarrow} C_n F_{2n+1} PO(OH)_2 \text{ or } (C_n F_{2n+1})_2 PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Major Commercial UsesMajor commercial UsesManeMasurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: 10% C_6 OFPIA, 3% C_6 Cs PFPIA, 5% C_{10} PFPA 37% C_6/C_6 PFPIA, 3% C_6 S PFPIA, 27% C_8/C_8 PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number52299-25-9Composition C_4/C_4 -PFPIA [3], [8]	Main Synthesis	Starting material: perfluoroalkyl iodides (PFA	Is, often as a mixture of linear homologs)
Then, eitherThen, either $C_nF_{2n+1}PI_2$ or $(C_nF_{2n+1})_2PI + H_2O$ $oxidant$ $C_nF_{2n+1}PO(OH)_2$ or $(C_nF_{2n+1})_2PO(OH)$ or $C_nF_{2n+1}PI_2$ or $(C_nF_{2n+1})_2PI + AgCl$ $oxidant$ $C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PCl$ $C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PCl + H_2O$ $oxidant$ $C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]ManeMasurf-780 [2]Composition 10% cs of PFPA, 8% Cs PFPIA, 5% C10 PFPA 37% Cs/Cs PFPIA, 33% Cs/Cs PFPIA, 27% Cs/Cs PFPIA $(amounting to 120\%, likely due to empirical deviations)$ NameTivida FL 2100 [3]CAS Number52299-25-9CompositionCu/Cq-PFPIA [3], [8]	Method [3]	$6 C_n F_{2n+1} I + P_4 \xrightarrow{heat} 2 C_n$	$F_{2n+1}PI_2 + 2(C_nF_{2n+1})_2PI$
$C_nF_{2n+1}Pl_2$ or $(C_nF_{2n+1})_2PI + H_2O \xrightarrow{oxidant} C_nF_{2n+1}PO(OH)_2$ or $(C_nF_{2n+1})_2PO(OH)$ or $C_nF_{2n+1}Pl_2$ or $(C_nF_{2n+1})_2PI + AgCl \xrightarrow{oxidant} C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PCl$ $C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PCl + H_2O \xrightarrow{oxidant} C_nF_{2n+1}PO(OH)_2$ or $(C_nF_{2n+1})_2PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably $n = 2$ or $n = 4$. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Major Commercial VeesMasurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: $10\% C_6$ PFPA, 8% C_8 PFPA, 5% C ₁₀ PFPA $37\% C_6/C_6$ PFPIA, 33% C ₆ /C_8 PFPIA, 27% C_8/C_8 PFPIA $(amounting to 120\%, likely due to empirical deviations)$ NameTivida FL 2100 [3]CAS Number52299-25-9CompositionC_4/C_4-PFPIA [3], [8]		Then, either	
oroxidantc_nF_{2n+1}Pl_2 or (C_nF_{2n+1})_2Pl + AgCloxidantC_nF_{2n+1}PCl_2 or (C_nF_{2n+1})_2PClC_nF_{2n+1}PCl_2 or (C_nF_{2n+1})_2PCl + H_2OoxidantC_nF_{2n+1}PO(OH)_2 or (C_nF_{2n+1})_2PO(OH)Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Industrial Practices & Commercial UsesMajor Commercial ProductsNameMasurf-780 [2]Omposition 10% C_6 PFPA, 8% C_8 PFPA, 5% C_10 PFPA 37% C_6/C_6 PFPIA, 33% C_6/C_8 PFPIA, 27% C_8/C_8 PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CanpositionCanposition [10% C_4-PFPIA [3], [8]		$C_n F_{2n+1} P I_2 \text{ or } (C_n F_{2n+1})_2 P I + H_2 O$	$\stackrel{nt}{\rightarrow} C_n F_{2n+1} PO(OH)_2 \text{ or } (C_n F_{2n+1})_2 PO(OH)$
$C_nF_{2n+1}PI_2$ or $(C_nF_{2n+1})_2PI + AgCl \xrightarrow{oxidant} C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PCl$ $C_nF_{2n+1}PCl_2$ or $(C_nF_{2n+1})_2PCl + H_2O \xrightarrow{oxidant} C_nF_{2n+1}PO(OH)_2$ or $(C_nF_{2n+1})_2PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably $n = 2$ or $n = 4$. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Industrial Practices & Commercial UsesMajor Commercial VersNameMasurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: 10% C_6 PFPA, 8% C_8 PFPA, 5% C_{10} PFPA 37% C_6/C_6 PFPIA, 33% C_6/C_8 PFPIA, 27% C_8/C_8 PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CompositionCu/C4-PFPIA [3], [8]		or	
$C_nF_{2n+1}PCl_2 \ or \ (C_nF_{2n+1})_2PCl + H_2O \xrightarrow{oxidant} C_nF_{2n+1}PO(OH)_2 \ or \ (C_nF_{2n+1})_2PO(OH)$ Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Industrial Practices & Commercial UsesMajor Commercial ProductsNameMasurf-780 [2]Composition $10\% C_6$ PFPA, 8% C_8 PFPA, 5% C_{10} PFPA $37\% C_6/C_6$ PFPIA, 33% C_6/C_8 PFPIA, 27% C_8/C_8 PFPIA $(amounting to 120\%, likely due to empirical deviations)$ NameTivida FL 2100 [3]Cas Number52299-25-9Composition C_4/C_4 -PFPIA [3], [8]		$C_n F_{2n+1} P I_2 \text{ or } (C_n F_{2n+1})_2 P I + Ag C I -$	$\xrightarrow{oxidant} C_n F_{2n+1} PCl_2 \text{ or } (C_n F_{2n+1})_2 PCl$
Alternatively, tri(perfluoroalkyl)difluorophosphoranes can be used as a starting material. This route then yields PFPIAs with side chains of the same length, preferably n = 2 or n = 4. [7]Possible ImpuritiesPFCAs and/or other byproducts can be formed during PFAI manufacture. [3]Industrial Practices & Commercial UsesMajor Commercial ProductsNameMasurf-780 [2]Composition 10% C6 PFPA, 8% C8 PFPA, 5% C10 PFPA 37% C6/C6 PFPIA, 33% C6/C8 PFPIA, 27% C8/C8 PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number52299-25-9CompositionC4/C4-PFPIA [3], [8]		$C_n F_{2n+1} PCl_2 \text{ or } (C_n F_{2n+1})_2 PCl + H_2 O$	$\stackrel{\text{lant}}{\longrightarrow} C_n F_{2n+1} PO(OH)_2 \text{ or } (C_n F_{2n+1})_2 PO(OH)$
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Major Commercise ProductsNameMasurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: 10% C6 PFPA, 8% C8 PFPA, 5% C10 PFPA 37% C6/C6 PFPIA, 33% C6/C8 PFPIA, 27% C8/C8 PFPIA 	Industrial Prac	tices & Commercial Uses	
NameMasurf-780 [2]Composition80% aqueous solution of mixtures of PFPAs and PFPIAs. [3] Measured composition: 10% C ₆ PFPA, 8% C ₈ PFPA, 5% C ₁₀ PFPA 37% C ₆ /C ₆ PFPIA, 33% C ₆ /C ₈ PFPIA, 27% C ₈ /C ₈ PFPIA (amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number52299-25-9CompositionC ₄ /C ₄ -PFPIA [3], [8]	Major Commer	cial Products	
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International Interna International International<	Composition	80% aqueous solution of mixtures of PFPAs a Measured composition:	nd PFPIAs. [3]
37% C ₆ /C ₆ PFPIA, 33% C ₆ /C ₈ PFPIA, 27% C ₈ /C ₈ PFPIA (amounting to 120%, likely due to empirical deviations) Name Tivida FL 2100 [3] CAS Number 52299-25-9 Composition C ₄ /C ₄ -PFPIA [3], [8]		10% C ₆ PFPA, 8% C ₈ PFPA, 5% C ₁₀ PFPA	
(amounting to 120%, likely due to empirical deviations)NameTivida FL 2100 [3]CAS Number52299-25-9CompositionC4/C4-PFPIA [3], [8]		37% C ₆ /C ₆ PFPIA, 33% C ₆ /C ₈ PFPIA, 27% C	8/C8 PFPIA
Name Tivida FL 2100 [3] CAS Number 52299-25-9 Composition C ₄ /C ₄ -PFPIA [3], [8]		(amounting to 120%, likely due to empirical d	leviations)
CAS Number 52299-25-9 Composition C ₄ /C ₄ -PFPIA [3], [8]	Name	Tivida FL 2100 [3]	
Composition C ₄ /C ₄ -PFPIA [3], [8]	CAS Number	52299-25-9	
	Composition	C ₄ /C ₄ -PFPIA [3], [8]	

Production or import volumes	EU: 0–10 t/yr [3	3], [8]			
Name	Phosphonic acid, perfluoro- C_{6-12} -alkyl derivatives (C_6 - C_{12} PFPAs) [3]				
CAS Number	68412-68-0				
Production or import volumes	US: <1,000,000 Denmark, Norw confidential bus) lbs (500t) in 2 ay, Sweden: >4 iness information	2015 [23] 4.33 t/yr in 199 on) [3]	9–2011 (some amounts have been claimed	l as
Name	Phosphinic acid	, bis(perfluoro-	C _{6–12} -alkyl) de	rivatives (C ₆ –C ₁₂ PFPIAs)	
CAS Number	68412-69-1				
Production or import volumes	US: <500t in 20 Denmark, Norw confidential bus)15 [23] ay, Sweden: >3 iness informatio	3.33 t/yr in 199 on) [3]	9–2011 (some amounts have been claimed	l as
Uses					
Major applications	Surfactants, leve textile industry,	elling and wetti pharmaceutical	ng agents in w industry, meta	axes and coatings, and defoaming agents in a lindustry, and in pesticide formulations [2]	in the 2], [9]
Regulatory Stat	us				
US	Some of these substances are regulated under 40 CFR §721.10536 Long-chain perfluoroalkyl carboxylate chemical substances [10]. A final rule to revoke the tolerance exemptions for mono- and bis- $(1H,1H,2H,2H)$ -perfluoroalkyl) phosphates (PAPs) where the alkyl group is even numbered and in the C ₆ -C ₁₂ range was published in August 2006 with an effective date 18 months after the publication of the final rule. They were used as surfactants (inert ingredients) in pesticide formulations in the past, but are no longer included in U.S. EPA's list of approved inert ingredients for pesticide				
Canada	As CAS Numbers 68412-68-0 and 68412-69-1 are also precursors to long-chain (C ₉ –C ₂₀) PFCAs, they were assessed together in 2012 and are managed pursuant to the <i>Prohibition of Certain Toxic Substances Regulations</i> , 2012 [19], [20].				
International ef	forts				
The proposal to I A, B and/or C to Organic Pollutan	ist long-chain per the Stockholm C ts Review Comm	fluorocarboxyli Convention on H ittee [22].	c acids (PFCA Persistent Orga	s), their salts and related compounds in Annic Pollutants is under review by the Pers	nexes
Examples of rej	ported occurren	ices			
Type of	(Environ-	Detected in	Examples		
locations/ samples	mental) media	one or multiple regions	Location, year	Levels [minmax. (detection frequency)]	Ref.
Note: Non-detect	s are reported as $NR - not$ report	below the value	e of the limit of	f detection (" <lod").< td=""><td></td></lod").<>	
Close to fluorochemical manufacturing park	air ≦ surface water Soil Sediment	\boxtimes one \square multiple \boxtimes one	China, 2012	C ₆ PFPA: <0.04–30.2 ng/L (2/32)	[13]
Close to			North	C ₆ PFPA: <0.025–1.2 ng/L (12/30)	[14]

ENV/CBC/MONO(2022)1 | 13

agricultural inputs	Surface water Soil Sediment	multiple	America, 2005 & 2007	C ₈ PFPA: <0.025–3.4 ng/L (24/30) C ₁₀ PFPA: <0.025–0.87 ng/L (22/30)	
Not close to specific point	☐ air ⊠ surface	one multiple	Europe, 2009	C ₈ PFPA: 1.0 ng/L (1/10)	[15]
sources	soil		Asia, 2009	C ₆ PFPA: <0.3–9.95 ng/L (14/76)	[16]
WWTP	⊠ effluent □ sludge	☐ one ⊠ multiple	North America, 2004 & 2007	C ₆ PFPA: <0.083–6.5 ng/L (4/7) C ₈ PFPA: <0.083–2.5 ng/L (6/7) C ₁₀ PFPA: <0.083–0.46 ng/L (3/7)	[14]
Indoor environment	Indoor dust	⊠ one □ multiple	North America, 2007–2008	C ₆ PFPA: <0.25-846 ng/g (57/102) C ₈ PFPA: <0.38-290 ng/g (28/102) C ₁₀ PFPA: <2.1-152 ng/g (6/102) C ₆ /C ₆ PFPIA: <0.088-525 ng/g (62/102) C ₆ /C ₈ PFPIA: <0.086-944 ng/g (78/102) C ₈ /C ₈ PFPIA: <0.17-525 ng/g (42/102)	[18]
Wildlife	Lake trout	☐ one ⊠ multiple	North America, 2008–2010	C ₆ /C ₆ PFPIA: <0.001–0.018 ng/g (NR) C ₆ /C ₈ PFPIA: <0.002–0.032 ng/g (NR)	[9]
	Double- crested cormorants		North America, 2010–2012	$\begin{array}{l} C_6/C_6 \ PFPIA: 0.2-1.6 \ ng/g \ ww \\ (grouped means, 66/66) \\ C_6/C_8 \ PFPIA: 0.25-3.0 \ ng/g \ ww \\ (grouped means, 66/66) \\ C_8/C_8 \ PFPIA: <0.025-0.29 \ ng/g \ ww \\ (grouped means, 55/66) \\ C_6/C_{10} \ PFPIA: $	[21]
Human	general population ccupational exposure	☐ one ⊠ multiple	North America, 2009	C ₆ /C ₆ PFPIA: <1–50.24 ng/g (17/70) C ₆ /C ₈ PFPIA: <1–60.96 ng/g (28/40) C ₈ /C ₈ PFPIA: <1–22.19 ng/g (1/40)	[17]
Knowledge gaps					
- Information on commercial products, especially current production and use (including volumes).					

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2. Perfluoroalkyl carboxylic (a) and dicarboxylic (b) acids

Key publication: Prevedouros, Konstantinos, Ian T. Cousins, Robert C. Buck, and Stephen H. Korzeniowski. 2006. "Sources, Fate and Transport of Perfluorocarboxylates." *Environmental Science & Technology* 40 (1): 32–44. https://doi.org/10.1021/es0512475.

Chemical Information & Properties				
Identification and T	Ferminology			
Name	Perfluoroalkyl carboxylic acids ⁵	Perfluoroalkyl dicarboxylic acids		
Other Names	Perfluorcarboxylic acids; perfluorinated carboxylic acids; perfluoroalkanoic acids [1]	Fluorinated dicarboxylic acids; perfluoroalkanedicarboxylic acids [2]		
Acronym	PFCAs	PFdiCAs		
Chemical Formula	$C_{(n-1)}F_{2n-1}COOH$	$C_{(n-2)}F_{2n-4}(COOH)_2$		
General Structure (linear isomers)		HO = F = O = O = O = O = O = O = O = O =		
US EPA CompTox Markush ID	DTXSID00893893	DTXSID80893896		
Individual acronyms and carbon chain length (as recommended by Buck et al. 2011)	Short-chain PFCAs (n ≤ 7) TFA: n=2; PFPrA: n=3; PFBA: n=4; PFPeA: n=5; PFHxA: n=6; PFHpA: n=7; Long-chain PFCAs (n ≥ 8) PFOA: n=8; PFNA: n=9; PFDA: n=10; PFUnDA: n=11: PFDoDA: n=12; PFTrDA: n=13; PFTeDA: n=14			
Degradability, Mob	oility, Bioconcentration			
Note: The following	information refers only to PFCAs, due to a lack	of information on PFdiCAs.		
Abiotic degradation	PFCAs generally do not undergo degradation ir	the environment [3].		
Atmospheric degradation	An estimated atmospheric lifetime regarding degradation (via reaction with OH radicals, forming COF_2) of PFCAs (n >1) is 130 days. Dry and wet deposition is more relevant, with time scales in the order of 10 days. [4]			
Biodegradation	No degradation of PFCAs under aerobic or anaerobic conditions over 15 weeks in closed bottle tests with municipal sewage sludge [5] ⁶			
Bioaccumulation potential	Long-chain PFCAs ($n \ge 8$) are known to be bioa proteinophilic nature and slow elimination rates	accumulative [9], [10]. Due to their s in air-breathing animals they are		

⁵ For more examples of compounds in the group of PFCAs and their associated information, one may search for "DTXSID40893892", "DTXSID00893893", "DTXSID60893894" at the U.S. EPA CompTox Chemicals Dashboard: <u>https://comptox.epa.gov/dashboard</u>.

⁶ One study found PFOA was no longer detected after 26 d under anaerobic conditions in WWTP sludge [6]. However, since no increase in fluoride concentration was observed, it is doubtful that this result is due to anaerobic degradation, and more likely to be due to sorption phenomena [7]. In another study, PFOA was found to be partially degraded (removal of up to 60% over 100 day inoculations) by a specific bacterial strain (Acidimicrobium sp. Strain A6) under laboratory conditions where they were used as the sole source of carbon; the applicability of this method in the field environment is currently unclear. [8]

	especially bioaccumulative in higher trophic level wildlife and humans [11]. Some short-chain PFCAs (such as PFBA and PFHxA) are also biomagnifying with BMF values >1 [11].
TMF (trophic magnification factor)	<i>In the overall Arctic marine food web</i> [12]: PFHpA: 0.76; PFOA: 1.93; PFNA: 4.23; PFDA: 4.81; PFUnDA: 4.79; PFDoDA: 2.96; PFTeDA: 1.97 <i>In French riverine systems</i> [13]: PFOA: 0.39–0.58; PFNA: 0.61–9.9; PFDA: 2.6–10.9; PFUnDA: 2.4, 42; PEDoDA: 1.4, 2.7; PETrDA: 0.9–14.9; PETrDA: 0.7, 2.8
BCF (carp, liver/blood, [L/kg]) ⁷ [14]	PFOA 134 / 611; PFNA: 150 / 4686; PFDA: 5957 / 34,896; PFUnDA: 1877 / 17,328; PFDoDA: 1945 / 11,988
Plant uptake	PFCAs have been found to accumulate in plants, with BCF values generally decreasing as chain lengths increase [61]–[64]. In various crops (lettuce, tomato, cabbage, zucchini), highest concentrations of long-chain PFCAs (> C_{11}) have been found in roots, while short-chain PFCAs have been found to accumulate in leaves. [61], [62] In trees (birch, spruce), the highest BCF values (chain-length-unspecified) have been
	found in foliage. [64]
Environmental transport	Main emissions sources of PFCAs lie in fluoropolymer manufacture and degradation of fluorotelomer compounds, among others [9]. Apart from manufacturing sites, relevant point sources also include airports, military bases, and other installations where AFFFs are or were used, as well as landfills. [15], [16]
	The majority of PFCAs in the environment are contained within the oceans, where sediment and the transport to deep oceans are sinks. Similarly, oceanic transport is believed to be most important transport pathway for PFCAs to the Arctic ocean. [3]
Adsorption on organic matter ⁸ (log K _{oc} , [log L/kg])	Log $K_{oc} = 2.1$ (for PFOA, average derived from multiple studies) [17]
Partition coefficients (K_d) between sediment and water	Increasing with chain length: 0.04 (PFOA)–0.72 (PFDoDA) [14] (measured in Korea, n=17)
Synthesis	
Main Synthesis Method	Mainly electrochemical fluorination of alkanoyl fluorides is employed to produce PFCAs (although in a mixture of linear and branched isomers): $C_nH_{2n+1}COF + (2n + 1)HF \longrightarrow C_nF_{2n+1}COF + (2n + 1)H_2$ Hydrolysis then yields the respective carboxylic acid. Yields decrease with increasing chain length, and when acid chlorides instead of acid fluorides are used. [1], [2], [18], [19] Alternatively, telomerization-based processes, followed by dehydroiodination and
	oxidation or direct carboxylation of the fluorotelomer iodide, to synthesize linear

⁷ Note that due to the acidic nature and the proteinophilic properties of PFCAs, BCFs are not necessarily accurate indicators of their overall biomagnification behavior in aquatic organisms. [11]

⁸ It should be noted that "the behaviour of PFASs in the environment is more complex than can be explained by a single soil or sediment property and it is not appropriate to express the sorption behaviour of these chemicals normalized over the OC content of the sorbent (Koc). An assessment of the published data has shown that neither OC, pH nor clay content alone could explain the sorption behaviour of the PFASs." [18]

	DEC As suid, and a start (as a start in la) and a shart start the start is a start in l (as		
	also the fact cards #7 on n:2 fluorotelomers). [1], [2], [18], [56]		
	$+Cr_2 O_7^{2-}$		
	$F(CF_2)_n I + CH_2 CH_2 \longrightarrow F(CF_2)_n CH_2 CH_2 I \longrightarrow F(CF_2)_n CHCH_2 \xrightarrow{Orog} (CF_2)_n COOH$		
	$F(CF_2)_n I + CO_2 + Zn - Cu \xrightarrow{(aq.) HCl} (CF_2)_n COOH$		
	On a laboratory scale, there are several other synthesis methods available, see [19, p. 1488].		
	PFOA is synthesized by direct oxidation of the corresponding iodide ($C_8F_{17}I$) using SO ₃ (or H_2SO_4) ⁹ , yielding $C_7F_{15}CO_2X$ [20].		
	PFdiCAs are generally synthesized via the electrochemical fluorination method, followed by hydrolysis, acidification, and extraction (similarly to for PFCAs above) [2], or are obtained from diiodoperfluoroalkanes [67]		
Possible Impurities	Electrochemical fluorination is not very selective and yields – besides the target compound – a number of linear, branched, or cyclic homologues. In the telomerization process, the purity of the product depends on the purity of the starting material.		
Industrial Practices & Commercial Uses			
Major Commercial	Products		
Name	Ammonium perfluorooctanoate (APFO)		
Chemical Formula	$NH_4^+ C_7 F_{15} COO^-$		
CAS Number	3825-26-1		
Use	As a processing aid in the dispersion process for production of fluoropolymers [1]; surfactant [1]		
Production/Import	Global (1999): approx. 260 t/yr [3]		
volumes ¹⁰	US (2015): <500t in 2015 [21]		
	Global (1951–2004): 3600–5700 t (estimated) [3]		
Name	Ammonium perfluorononanoate (APFN)		
Chemical Formula	$NH_4^+ C_8F_{17}COO^-$		
CAS Number	4149-60-4		
Use	Processing aid in polyvinylidene fluoride (PVDF) production. [3]		
Production/Import volumes	Global (1951–2004): 800–2300 t (estimated) [3] Global (2004): 15–75 t/yr [3]		
Name	Surflon® S-111 [1], [3]		
Composition	74% APFN (NH ₄ ⁺ C ₈ F ₁₇ COO ⁻), 20% APFUnD (NH ₄ ⁺ C ₁₀ F ₂₁ COO ⁻), 5% APFTrD (NH ₄ ⁺ C ₁₂ F ₂₅ COO ⁻), 1% other linear PFCAs (with n=7,9,11) [1]		
CAS Number	72968-38-8		

⁹ According to information provided by representatives of the manufacturing industry.

¹⁰ Long-chain PFCAs have largely been phased out and replaced in the past years; however, no information on more recent production volumes is available.

Use	Processing aid in polyvinylidene fluoride (PVDF) production. [3]
Uses	
Major applications	PFCAs have been used as polymerization aids in the production of fluoropolymers, as surfactants, in insecticide formulations, and in various consumer products. Historically, PFCAs were also ingredients of early generations of fire-fighting foams [9], [23], [24].
	The use of silver salts of PFdiCAs in coordination polymers has been investigated [25], [26] and perfluoroadipic acid (HOOC–C ₄ F ₈ –COOH; CAS Number 336-08-3) is mentioned in a small number of patents (e.g. for thermoplastic elastomers or low-refractive-index layers in electrooptical devices) [27], [28]. PFdiCAs are also used to produce the corresponding alcohols via reduction [2].
	Perfluorosuccinic acid (377-38-8), perfluoroglutaric acid (376-73-8), and perfluoroadipic acid (336-08-3) are listed as commercially <i>active</i> in the US TSCA Inventory, while their uses are unknown.
Regulatory Status	
General remarks	Most risk assessment activities focus mainly on PFOA, the most prominent PFCA [18]. Furthermore, regulations generally focus more on longer-chain PFCAs ($n \ge 8$), and less on short-chain PFCAs, which are believed to be less bioaccumulative (although this belief is being challenged [10]) and are often used as replacement chemicals [10], [18], [29]. Many limit values for different environmental media have been set at regional, country and sub-country levels, and a comprehensive overview is available online by the US Interstate. Tashnology, Pagulatory, Council (ITPC), at https://pfog.l.itemuch.org/foot
	<u>sheets/</u> (see "PFAS Water and Soil Values Table"). [30]
US	Under the 2010/2015 PFOA Stewardship Program by the U.S. EPA, eight major multi- national fluoropolymer and fluorotelomer manufacturers started to phase out long-chain PFCAs in 2006, which was achieved by 2015. [32] In July 2020, U.S. EPA issued a final rule requiring notice and U.S. EPA review before manufacturing/processing of certain long-chain PFAS that have been phased out in the United States could commence. [32] In March 2020, U.S. EPA made a preliminary determination to regulate PFOA in drinking water. U.S. EPA finalized regulatory determinations in February 2021. In addition, certain PFCAs are regulated at the state level in the United States. [33]
Europe	PFOA and its ammonium salt (APFO), as well as C_9-C_{14} PFCAs have been identified as substances of very high concern (SVHCs) under REACH in 2013 [34]. PFOA, APFO and related substances have been also added to the restricted substances list (REACH Annex XVII) in 2017. Restrictions of PFHxA, C_9-C_{14} PFCAs and related substances have also been proposed [35], [36]. In summer 2020, PFOA and related compounds moved to the EU POP regulation [37]. EFSA set a TWI (tolerable week intake) value for PFOA of 6 ng/kg bw (nanogram per kilogram bodyweight) in 2018 [18] and in 2020 set a TWI value for the sum of PFOA, PFNA, PFHxS and PFOS of 4.4 ng/kg bw [38].
Canada	PFOA, its salts and precursors as well as long-chain perfluorocarboxylic acids (LC-PFCAs), their salts and precursors were assessed in 2012. [39], [40] These substances are prohibited with a limited number of exemptions under the <i>Prohibition of Certain Toxic Substances Regulations</i> , 2012 [41].
International Effor	ts
PFOA, its salts, and	PFOA-related compounds are listed as POPs (persistent organic pollutants) under the

Annex A (Elimination) to the Stockholm Convention, with several specific exemptions [31]. See the listing for the definition of PFOA-related compounds covered.

In 2021, long-chain PFCAs (C_9-C_{21}), their salts and related compounds were proposed for listing under the Stockholm Convention (see UNEP/POPS/POPRC.17/7 at <u>https://www.pops.int/poprc17</u>).

Examples of reported occurrences					
Type of	(Environ-	Detected in	Examples		
locations/ samples	mental) media	one or multiple regions	Location, year	Levels [min. –max. (detection frequency)]	Ref.
Note: Non-detects are reported as below the value of the limit of detection (" $").ng = nanograms$, $dw = dry$ weight, $ww = wet$ weight, $ND = not$ detected, $NR = not$ reported					
Close to fluorochemical manufacturing	☐ air ⊠ surface water ☐ soil	☐ one ⊠ multiple	Europe, 2016	PFBA: 4.6–12.0 ng/L (13/13) PFPeA: <4–8.2 ng/L (10/13)	[42]
park or other point sources	sediment sediment			PFHxA: 4–6.4 ng/L (13/13) PFHpA: 1.5–2.2 ng/L (13/13) PFOA: 3.5–12 ng/L (13/13)	
				PFNA: 0.49–1.0 ng/L (13/13) PFDA: 0.23–0.8 ng/L (13/13)	
	i air surface water soil sediment Earth worm	☐ one ☐ multiple ☐ one ☐ multiple	North America, 2009 North America,	PFHpA: 0.88–6.6 ng/g dw (19/19) PFOA: 47–470 ng/g dw (19/19) PFNA: 1.6–6.3 ng/g dw (19/19) PFDA: 2.1–5.3 ng/g dw (19/19) PFUnDA: 2.6–14 ng/g dw (19/19) PFDoDA: 2.2–11 ng/g dw (19/19) PFHpA: ND–3.6 ng/g dw (14/19) PFOA: 51–860 ng/g dw (19/19)	[43]
			2009	PFNA: 2.0–52 ng/g dw (19/19) PFDA: 5.9–74 ng/g dw (19/19) PFUnDA: 19–380 ng/g dw (19/19) PFDoDA: 22–660 ng/g dw (19/19)	
	Surface water, groundwater, waste leachate	⊠ one □ multiple	Sweden, 2017– 2018	TFA: <34–14000 ng/L (21/34) PFPrA: <3.1–53000 ng/L (27/34)	[60]
Not close to specific point sources	☐ air ⊠ surface water ☐ soil ☐ sediment	☐ one ⊠ multiple	Asia, 2010 & 2012	PFHxA: ND-7.94 ng/L (15/19) PFHpA: ND-3.43 ng/L (16/19) PFOA: ND-8.34 ng/L (17/19) PFNA: ND-4.49 ng/L (16/19) PFDA: ND-4.80 ng/L (12/19) PFUnDA: ND-1.13 ng/L (15/19)	[14]

				PFDoDA: ND-0.33 ng/L (12/19)	
	Drinking water ¹¹	☐ one ⊠ multiple	Europe,	PFBA <2-13 ng/L (1/6)	[42]
			2016	PFPeA: <4–5.7 ng/L (2/6)	
				PFHxA: <0.1–5.3 ng/L (5/6)	
				PFHpA: <0.05-2.4 ng/L (3/6)	
				PFOA: <0.3–2.7 ng/L (4/6)	
				PFNA: <0.03-0.28 ng/L (3/6)	
				PFDA: <0.03–0.1 ng/L (2/6)	
			Canada	PFBA <1-10 ng/L (151/226)	[55]
			2012-	PFPeA: <1–15 ng/L (115/226)	
			2019	PFHxA: <1–13 ng/L (122/226)	
				PFHpA: <1–3.6 ng/L (27/226)	
				PFOA: <0.5–7.6 ng/L (165/226)	
				PFNA: <0.5–1.2 ng/L (41/226)	
				PFDA: <0.5–0.63 ng/L (5/226)	
				PFUnDA: <1 ng/L (0/226)	
				PFDoDA: <1 ng/L (0/226)	
	DWTP influent		North	PFBA: <0.24–96.8 ng/L (23/25)	[44]
			America, 2013– 2015	PFPeA: <0.051–501 ng/L (23/25)	
				PFHxA: <0.044–55.1 ng/L	
				(24/25) PEHpA: <0.04-184 pg/L (24/25)	
				PFOA: <0.56–112 ng/L (19/25)	
				PFNA: <0.094–41.4 ng/L (24/25)	
				PFDA: <0.084-31.1 ng/L (15/25)	
				PFUnDA: <0.067–2.9 ng/L (8/25)	
				PFDoDA: <0.062–0.28 ng/L	
				(2/23) PFTrDA: <0.072 ng/L (0/25)	
				PFTeDA: <0.13 ng/L (0/25)	
				PFHxDA: <0.4 ng/L (0/25)	
				PFOcDA: <0.29 ng/L (0/25)	
	DWTP effluent			PFBA: <0.24–104 ng/L (22/25)	[44]
				PFPeA: $<0.051-514$ ng/L (24/25)	
				$\Gamma \Gamma \Pi XA: \Pi K = 00.8 \Pi g/L (23/23)$ PFHnA: <0.04=177 ng/L (23/25)	
				1111p11. < 0.07 177 112(23/23)	

¹¹ U.S. EPA has also collected nationwide drinking water data for certain PFAS, a summary of which can be found here: <u>https://www.epa.gov/sites/production/files/2017-02/documents/ucmr3-data-summary-january-2017.pdf</u>. Such data were further analyzed in, e.g., Guelfo, J.L. and D.T. Adamson. 2018. "Evaluation of a national data set for insights into sources, composition, and concentrations of per- and polyfluoroalkyl substances (PFASs) in U.S. drinking water." *Environmental Pollution* 236 (May): 505-513. Additionally, many U.S. states have also published data on the occurrence of PFAS in drinking water on their websites. Such data were recently analyzed in Andrews, D.Q. and Naidenko, O.V. 2020. Population-wide exposure to per- and polyfluoroalkyl substances from drinking water in the United States. *Environmental Science & Technology Letters* 7(12): 931–936.

	□ air □ surface water □ soil ⊠ sediment	☐ one ⊠ multiple	Asia, 2010 & 2012	PFOA: <0.56–104 ng/L (19/25) PFNA: <0.094–38.6 ng/L (22/25) PFDA: <0.084–24.7 ng/L (13/25) PFUnDA: <0.067–1.85 ng/L (4/25) PFDoDA: <0.062–0.09 ng/L (1/25) PFTrDA: <0.072 ng/L (0/25) PFTeDA: <0.13 ng/L (0/25) PFHxDA: <0.4 ng/L (0/25) PFOcDA: <0.29 ng/L (0/25) PFHxA: ND–0.05 ng/g dw (6/27) PFHpA: ND–0.06 ng/g dw (3/27) PFOA: ND–0.28 ng/g dw (24/27) PFNA: ND–0.15 ng/g dw (24/27)	[14]
				PFDA: ND-0.08 ng/g dw (24/27) PFDoDA: ND-0.09 ng/g dw (24/27) PFDoDA: 0.01-0.13 ng/g dw (23/27) PFUnDA: 0.01-0.13 ng/g dw (27/27)	
	Snow (ski area)		Northern Europe, 2010	PFHxA: <4.0–15.9 ng/L (7/8) PFHpA: <13.3 ng/L (0/8) PFOA: <7.8–55.5 ng/L (6/8) PFNA: <11.2–19.6 ng/L (1/8) PFDA: <4.15–17.2 ng/L (6/8) PFUnDA: <3.16–12.8 ng/L (5/8) PFDoDA: <0.168–21.8 ng/L (7/8) PFTrDA: <1.72–22.0 (6/8) PFTeDA: <0.377–57.9 (7/8) PFPeDA: <0.615–16.8 ng/L (5/8) PFHxDA: <1.36–108 ng/L (5/8) PFHpDA: <1.4–55.9 ng/L (4/8) PFOcDA: <4.03–60.6 ng/L (3/8) PFEiA: <3.29–113 ng/L (4/8)	[45]
Remote regions	Ice (41 cm depth)	☐ one ⊠ multiple	Arctic, 2017	TFA: 137 ng/L (1/1) PFPrA: 6.3 ng/L (1/1) PFBA: 1.5 ng/L (1/1)	[46]
WWTP	⊠ effluent □ sludge	☐ one ⊠ multiple	Europe, 2007	PFPeA: 1.5–40.9 ng/L (9/9) PFHxA: 3.7–57.4 ng/L (9/9) PFHpA: 1.6–15.7 ng/L (9/9) PFOA: 12.3–77.6 ng/L (9/9) PFNA: 1.0–18.6 ng/L (9/9) PFDA: 0.9–34.5 ng/L (9/9)	[47]

				PFUnDA: <0.004-8.8 ng/L (7/9)	
				PFDoDA: <0.01–0.5 ng/L (3/9)	
	S effluent	one	United	PFHxA: 3.67–99.0 ng/L (28/28)	[57]
	sludge	⊠ multiple	States,	PFHpA: ND-12.9 ng/L (27/28)	
			2012 & 2013	PFOA: 5.70–38.8 ng/L (28/28)	
			2010	PFNA: 0.83–4.95 ng/L (28/28)	
				PFDA: 1.11–4.43 ng/L (28/28)	
				PFUnDA: ND-0.92 ng/L (16/28)	
				PFDoDA: ND-5.91 ng/L (9/28)	
Landfill		one	Canada,	PFBA: NR-0.29 μg/L	[58]
leachate and		M multiple	2021	PFPeA: NR-0.21 µg/L	
aroundwater				PFHxA: NR–0.67 µg/L	
(historic =				PFHpA: NR-0.27 µg/L	
closed 25-90				PFOA: NR–0.85 µg/L	
years)				PFNA: NR-1.0 µg/L	
				PFDA: NR-0.006 μg/L	
				PFUnA: NR-0.016 µg/L	
				PFDoDA: NR-0.001 µg/L	
				PFTriDA: NR-0.007 µg/L	
				PFTeDA: NR-0.0002 µg/L	
Indoor environment	Indoor air (hotel rooms)	☐ one ⊠ multiple	Asia, 2015	C ₄ C ₇ -PFCAs: 0.04440.541 ng/m ³ (13/13)	[48]
				> C ₇ -PFCAs: 0.0568–0.756 ng/m ³ (13/13)	
	Indoor air (residential			C ₄ -C ₇ -PFCAs: 0.351-1.970 ng/m ³ (19/19)	
	homes)			> C7-PFCAs: 0.091–0.686 ng/m ³ (19/19)	
	Indoor dust (hotel rooms)			C4–C7-PFCAs: ND–170 ng/g (7/13)	
				> C ₇ -PFCAs 11.5–775 ng/g (13/13)	
	Indoor dust (residential			C4-C7-PFCAs: 41.6-226 ng/g (19/19)	
	homes)			> C ₇ -PFCAs: 10.7–205 ng/g (19/19)	
Vegetation	Tree leaves	one	North	PFHpA: 2.4–7.3 ng/g dw (19/19)	[43]
		M multiple	America,	PFOA: 200–700 ng/g dw (19/19)	
			2009	PFNA: 0.36–5.8 ng/g dw (19/19)	
				PFDA: 1.2–4.3 ng/g dw (19/19)	
				PFUnDA: 1.6–8.6 ng/g dw	
				(19/19)	

				PFDoDA: <0.216–4.2 ng/g dw (15/19)	
Wildlife	Plankton	one	Asia, 2010 & 2012 ¹²	PFNA: ND-0.50 ng/g ww (10/12)	[14]
		X] multiple		PFDA: ND-0.39 ng/g ww (1/12)	
				PFUnDA: ND-0.44 ng/g ww (6/12)	
				PFDoDA: ND-1.08 ng/g ww (7/12)	
	Crucian carp,		Asia,	PFHxA: ND-0.36 ng/ml (7/69)	[14]
	blood		2010 &	PFOA: ND-0.89 ng/ml (24/69)	
			2012	PFNA: ND-13.22 ng/ml (16/69)	
				PFDA: 0.44–20.58 ng/ml (69/69)	
				PFUnDA: 0.88–45.16 ng/ml (69/69)	
				PFDoDA: 0.11–19.18 ng/ml (69/69)	
	Crucian carp,		Asia, 2010 & 2012	PFOA: ND-0.33 ng/g ww (9/69)	[14]
	liver			PFNA: ND-0.86 ng/g ww (30/69)	
				PFDA: 0.06–3.48 ng/g ww (69/69)	
				PFUnDA: 0.04–5.01 ng/g ww (69/69)	
				PFDoDA: ND–2.08 ng/g ww (67/69)	
	Peregrine falcons, plasma	⊠ one □ multiple	Canada, 2016 & 2018	PFBA: ND-6.70 ng/g ww (5/57) PFPeA: ND-0.23 ng/g ww (3/57) PFHxA: ND-3.56 ng/g ww (41/57) PFHpA: ND-3.14 ng/g ww (28/57) PFOA: 0.17-2.38 ng/g ww (57/57) PFNA: 0.83-21.8 ng/g ww (57/57) PFDA: 0.45-9.65 ng/g ww (57/57) PFUnDA: 0.78-9.84 ng/g ww (57/57) PFDoDA: 0.24-3.62 ng/g ww (57/57) PFTrDA: 0.56-4.49 ng/g ww (57/57) PFTeDA: 0.22-2.81 ng/g ww (57/57)	[59]

¹² PFHxA, PFHpA, and PFOA were not detected in any sample.

				PFHxDA: 0.09–3.00 ng/g ww (55/57) PFODA: 0.01–1.08 ng/g ww (18/57)	
	Peregrine falcons, egg	⊠ one ☐ multiple	Canada, 2018	PFBA: ND ng/g ww (0/9) PFPeA: ND-0.64 ng/g ww (8/9) PFHxA: 0.06-0.09 ng/g ww (9/9) PFHpA: ND-0.06 ng/g ww (9/9) PFOA: 0.11-0.31 ng/g ww (9/9) PFOA: 0.46-4.05 ng/g ww (9/9) PFDA: 0.90-3.49 ng/g ww (9/9) PFUnDA: 1.12-7.22 ng/g ww (9/9) PFDoDA: 1.47-4.05 ng/g ww (9/9) PFTrDA: 1.93-8.18 ng/g ww (9/9) PFTeDA: 1.40-5.25 ng/g ww (9/9) PFHxDA: 0.19-0.46 ng/g ww (9/9)	
Human serum	general population ccupational exposure	one Multiple	Asia, 2011	PFODA: ND-0.03 ng/g ww (7/9) TFA: 5.36-12.55 ng/ml (244/252) PFPrA: 0.24-0.82 ng/ml (194/252) PFBA: 0.31-0.89 ng/ml (216/252) PFHxA: 0.41-0.76 ng/ml (251/251) PFHpA: ND-0.18 ng/ml (168/252) PFOA: 8.45-26.76 ng/ml (252/252) PFNA: 1.99-5.20 ng/ml (252/252) PFDA: 0.96-4.11 ng/ml (250/252) PFUnDA: 1.71-3.02 ng/ml (252/252) PFDoDA: 0.07-0.21 ng/ml (224/252)	[49]
	general population ☐ occupational exposure		Canada, 2016- 2017	PFOA: 1.3 ng/ml (mean; 2593/2593) PFNA: 0.51 ng/ml (mean; 2413/2442) PFDA: 0.18 ng/ml (mean; 2157/2360)	[65]
	general population ccupational exposure		North America, 2015–	PFNA: 0.577 ng/ml (mean; NR/1993) PFDA: 0.154 ng/ml (mean; NR/1993)	[66]

	2016	PFOA: 1.56 ng/ml (mean; NR/1993)	
Children age 3- 11	North America, 2013– 2014	PFOA (linear): <0.07-8.22 ng/ml (638/639) PFOA (branched): <0.07-0.69 ng/ml (163/639) PFHpA: <0.07-0.97 ng/ml (124/639) PFNA: <0.07-52.92 ng/ml (638/639) PFDA: <0.07-2 ng/ml (300/639) PFUnDA: <0.07-2.83 ng/ml (208/639) PFDoDA: <0.07 ng/ml (0/639)	[50]

Other known occurrences and sources

Many other PFASs, such as fluorotelomer-based substances, can yield PFCAs upon degradation, including atmospheric oxidation of volatile precursors [9], [51], [52], [54]. For example, degradation (e.g. via OH-radicals) of fluoroalkylsilane substances can yield significant amounts of PFCAs [53].

Knowledge gaps

- Little is known about the uses, occurrence, and environmental fate of PFdiCAs.

- Current production volumes of PFCAs and PFdiCAs are unknown.

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Chemical Information & Properties Identification and Terminology¹³ Perfluoroalkane sulfinic acids Name Perfluoroalkane sulfonic acids Other Names Perfluoroalkyl sulfonic acids; Perfluoroalkyl sulfinic acids; fluorinated alkanesulfinic acids fluorinated alkanesulfonic acids Acronym PFSAs PFSIAs Chemical Formula $C_n F_{2n+1} SO_2 OH$ $C_n F_{2n+1} SOOH$ General Structure *(linear isomers)* ОН DTXSID70892979 DTXSID801024681 US EPA CompTox Markush ID Individual *Short-chain PFSAs (n* ≤5): PFBS: n=4; PFPeS: n=5 PFOSI: n=8 (other PFSIAs exist. but no information on those was Acronyms (as used Long-chain PFSAs ($n \ge 6$): PFHxS: n=6; PFHpS: *in this document*) n=7; PFOS: n=8; PFNS: n=9; PFDS: n=10 available) Degradability, Mobility, Bioconcentration General remarks PFOS and other long-chain PFSAs are known to be PFSIAs are transformed to PFSAs bioaccumulative and persistent in the environment in the environment. [3] [1], with PFHxS being the most bioaccumulative PFAS known [2]. Short-chain PFSAs ($n \le 5$) are less bioaccumulative, but are expected to be of similar persistence [1], [4]. **Photochemical** PFOS photolyzes slowly under UV C light (100-280 nm), with complete degradation in 11 days [5]. degradation *Hydrolysis* PFOS hydrolyzes at high temperatures (300 °C) [6]. No biodegradation of PFOS observed [7]. **Biodegradation** PFSAs are not effectively removed by conventional activated sludge processes in WWTP [8], [9].¹⁴ $Log K_{oc} = 2.68$ (PFOS, in sediment) [10] Adsorption on organic matter $(\log K_d, cm^3/g)$ Partition 0.03 (PFHxS); 0.07 (PFOS) [11] coefficients (K_d , (measured in Korea, n=17) sediment-water)

3. Perfluoroalkane sulfonic (a) and sulfinic (b) acids

¹³ For more examples of compounds in the group of PFSAs and their associated information, one may search for "DTXSID70892979" at the U.S. EPA CompTox Chemicals Dashboard: https://comptox.epa.gov/dashboard ¹⁴ In one study, PFOS was found to partially degraded (removal of up to 60% over 100 day inoculations) by a specific bacterial strain (Acidimicrobium sp. Strain A6) under laboratory conditions where they were used as the sole source of carbon; the applicability of this method in the field environment is currently unclear. [56]

Bioaccumulation potential	PFOS: depuration half-life (rainbow trout) = 13d Blood elimination half-life (rat, male) = 8–30d [7] Short-chain PFSAs (PFBS) are accumulating in plants and trees [12-15]. In various crops (lettuce, tomato, cabbage, zucchini) PFBS and PFHxS accumulate rather in leaves, whereas PFOS accumulates rather in roots. In trees (birch, spruce), the highest BCF values have been found in foliage. [56]–[59]	
<i>TMF in the overall</i> <i>Arctic marine food</i> <i>web</i> [16]	PFOS: 17.4	
TMF in riverine systems [17]	PFHxS: 0.36–3.7 PFHpS: 0.65–8.3 PFOS (linear): 0.81–4.5 PFOS (branched): 1.4–8.3 PFDS: 0.73–3.0	
BAF (earthworm)	PFBS: 0.21–0.92 PFHxS: 0.51–4.69 [18]	
BMF (different species)	PFHxS: 6.9–22 [19]; 20 [20] PFOS: 30 [20] PFDS: 36 [20]	
BCF ¹⁵ (carp, liver/blood, [L/kg])	PFHxS: 8 / 342 PFOS: 4572 / 11,167 [11]	
Synthesis		
Main Synthesis Method	Mostly the Simons electrochemical fluorination proc sulfonyl fluoride is electrolyzed in anhydrous hydrog $C_nH_{2n+1}SO_2F + (2n + 1)HF \longrightarrow C_nF_2$ Alternatively, a nonelectrochemical route for the sy acid derivatives is also possible: $F_3C - S - S - CF_3 \xrightarrow{Cl_2} 2F_3C - S - C$ Alkaline hydrolysis then gives the sulfonate salt, whi	cess is used, where the hydrocarbon gen fluoride: $2n+1SO_2F + (2n + 1)H_2$ where the hydrocarbon control $Cl \xrightarrow{Cl_2}{H_2O} 2F_3C - SO_2Cl$ ich can be acidified to yield the acid.
	PFSIAs are similarly also synthesized via electroche	mical fluorination [1].
Possible Impurities	The electrochemical fluorination process is unseled compound, a mixture of linear, branched, and cyclic impurities in the final product [1], [22]. Product yie lengths [23].	ctive and yields, besides the target homologues, which can be found as elds decrease with increasing chain

¹⁵ Note that due to the acidic nature and the proteinophilic properties of PFSAs, BCFs are not necessarily accurate indicators of their overall biomagnification behavior in aquatic organisms. [10]

Industrial Practices	& Commercial Uses
Major Commercial I	Products
Name	Perfluorooctane sulfonic acid (PFOS)
CAS Number	1763-23-1
Production/Import volumes	PFOS production was phased out in the US (in 2002), but it is still being produced in China. The production volume of perfluorooctane sulfonyl fluoride (the parent compound of PFOS) in China in 2006 was more than 200 tonnes [1]. Global production between 2003 and 2008 reached 410 tonnes, mainly in China, followed by Japan and Germany [24]. Production volumes in 2015 were estimated at 170 tonnes per year in China [25].
Uses	Surfactant [1] (e.g. potassium salt of PFOS, CAS Number 2795-39-3, as a mist suppressant in electroplating) [24]
Name	Potassium perfluorobutanesulfonate (K-PFBS)
CAS Number	29420-49-3
Production/Import volumes	Registered under REACH with a production/import volume of 100–1000 tonnes/yr in Europe. [26]
Uses	Mainly used as flame retardant in polycarbonate, but also as intermediate in the synthesis of other chemicals. [27]
Uses	
Major applications	Short-chain PFSAs are used as esterification catalysts, as electrolytes in fuel cells and batteries (in the form of their lithium salts), as antistatic agents, and as flame retardants (K-PFBS is mainly used as flame retardant in polycarbonate) [27], [21]. Longer-chain PFSAs are used as surfactants and in fire extinguishing formulations [21]. PFSIAs themselves are not commercially used, but are known degradation products formed from perfluoroalkane sulfonamides. [1]
Regulatory Status	
General remarks	Current risk assessment and regulations mainly focus on PFHxS and PFOS, with short- chain PFSAs such as PFBS being used as replacements [4], [22]. Many limit values for different environmental media have been set at regional, country and sub-country levels, and a comprehensive overview is available online by the US Interstate Technology Regulatory Council (ITRC) at <u>https://pfas-1.itrcweb.org/fact-</u> <u>sheets/</u> (see "PFAS Water and Soil Values Table"). [28]
US	Through its voluntary agreement with US EPA, 3M (the then largest manufacturer) phased out its global production of PFOS in 2002. [32] US EPA promulgated Significant New Use Rules (SNURs) in 2002 and 2007 under the Toxic Substances Control Act (TSCA) that require manufacturers (including importers) and processors to notify US EPA at least 90 days before starting or resuming manufacture, import, or processing for significant new uses of 271 PFSAs and related compounds, essentially encompassing all PFSAs and related compounds on the US market. Articles (except carpets) containing these substances may still be imported. [33] In March 2020, US EPA made a preliminary determination to regulate PFOS in drinking water. US EPA finalized regulatory determinations in February 2021. In addition, certain PFSAs have been regulated at the state level in the US. [34]
Canada	PFOS, its salts and precursors were assessed in 2006 and are prohibited with a limited number of exemptions under the <i>Prohibition of Certain Toxic Substances Regulations</i> , 2012 [35], [36].

Europe	PFOS added	to the restricted	substances list	(REACH Annex XVII) in 2017 [37]				
1	In 2018, EFS 2020, EFSA s bw [39].	In 2018, EFSA set the tolerable week intake (TWI) for PFOS to 13 ng/kg bw [38] and in 2020, EFSA set a TWI value for the sum of PFOA, PFNA, PFHxS and PFOS of 4.4 ng/kg bw [39].						
	The EU Wate	The EU Water Framework Directive set an EQS (environmental quality standard) value						
	for PFOS (an	for PFOS (and its derivatives) in surface waters of 0.65 ng/L [40].						
PFBS and PFHxS (and their salts) are identified as SVHCs [41], [42].								
International ef	forts							
2002: OECD cla	ssified PFOS as a Pl	BT chemical. [2	9]					
2009: PFOS, its Convention as p amended in 2019	2009: PFOS, its salts and perfluorooctane sulfonyl fluoride added to Annex B (Restriction) to the Stockholm Convention as persistent organic pollutants (POPs) [53], with specific exemptions and acceptable purposes amended in 2019 [54].							
2013: Perfluoro perfluorooctane Procedure for Ce	ooctane sulfonic sulfonyls added to rtain Hazardous Che	acid, perfluoro Annex III to the emicals and Pes	boctane sulfor he Rotterdam ticides in Inter	nates, perfluorooctane sulfonamide Convention on the Prior Informed (national Trade. [55]	es and Consent			
PFHxS, its salts Committee (POF Conference of th	and related comp PRC) to the Stockhor e Parties (COP) in 2	oounds are reco olm Convention 022). [30], [31]	ommended by for listing unc	the Persistent Organic Pollutants ler the Convention (to be determined	Review l by the			
Examples of re	ported occurrence	es						
Type of	(Environmental)	Detected in	Examples					
locations/ samples	media	one or multiple regions	Location, year	Levels [min. –max. (detection frequency)]	Ref.			
Note: Non-detects are reported as below the value of the limit of detection (" $").pg = picograms, ng = nanograms, dw = dry weight, ww = wet weight, ND = not detected, NR = not reported$								
pg = picograms,	s are reported as be ng = nanograms, d	elow the value og w = dry weight,	f the limit of de ww = wet wei	etection (" <lod"). ght, ND = not detected, NR = not rep</lod"). 	orted			
pg = picograms, Close to	is are reported as being = nanograms, d	$w = dry \ weight,$ one	f the limit of deww = wet weigNetherlands	etection (" <lod"). $ght, ND = not \ detected, \ NR = not \ rep$ PFBS: 16–27 ng/L (13/13)</lod"). 	orted [43]			
<i>pg = picograms,</i> Close to fluorochemical	is are reported as be ng = nanograms, d air surface water soil	$w = dry \ weight,$	f the limit of deww = wet weizNetherlands2016	etection (" <lod"). ght, ND = not detected, NR = not rep PFBS: 16–27 ng/L (13/13) PFHxS: 1.5–2.2 ng/L (13/13)</lod"). 	orted [43]			
Note: Non-delect pg = picograms, Close to fluorochemical manufacturing park	is are reported as be ng = nanograms, dr air surface water soil sediment	$ \begin{array}{c} clow the value of \\ w = dry weight, \\ \hline \\ \hline \\ one \\ \hline \\ \hline \\ \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	f the limit of de ww = wet wei Netherlands 2016	etection (" <lod"). ght, ND = not detected, NR = not rep PFBS: 16–27 ng/L (13/13) PFHxS: 1.5–2.2 ng/L (13/13) PFHpS: 0.095–0.2 ng/L (13/13)</lod"). 	orted [43]			
Note: Non-delect pg = picograms, Close to fluorochemical manufacturing park	is are reported as be ng = nanograms, dv air surface water soil sediment	Plow the value of $w = dry \ weight$, $w = dry \ weight$,	f the limit of de ww = wet weig Netherlands 2016	etection (" <lod"). ght, ND = not detected, NR = not rep PFBS: 16–27 ng/L (13/13) PFHxS: 1.5–2.2 ng/L (13/13) PFHpS: 0.095–0.2 ng/L (13/13) PFOS: 2.7–6.5 ng/L (13/13)</lod"). 	orted [43]			
Note: Non-detect pg = picograms, Close to fluorochemical manufacturing park Not close to	s are reported as be ng = nanograms, dr air surface water soil sediment	Plow the value of $w = dry \ weight$, \square one \square multiple \square one	f the limit of de ww = wet wei Netherlands 2016 Korea	etection (" <lod"). ght, ND = not detected, NR = not rep PFBS: 16–27 ng/L (13/13) PFHxS: 1.5–2.2 ng/L (13/13) PFHpS: 0.095–0.2 ng/L (13/13) PFOS: 2.7–6.5 ng/L (13/13) PFHxS: ND–3.97 ng/L (18/19)</lod"). 	orted [43] [11]			
Note: Non-delect pg = picograms, Close to fluorochemical manufacturing park Not close to specific point sources	s are reported as be ng = nanograms, dv air surface water soil sediment air surface water soil surface water soil	Plow the value of $w = dry \ weight$, \square one \square multiple \square one \square one \square multiple	f the limit of de ww = wet weig Netherlands 2016 Korea 2010 & 2012	etection (" <lod"). ght, ND = not detected, NR = not rep PFBS: 16–27 ng/L (13/13) PFHxS: 1.5–2.2 ng/L (13/13) PFHpS: 0.095–0.2 ng/L (13/13) PFOS: 2.7–6.5 ng/L (13/13) PFHxS: ND–3.97 ng/L (18/19) PFOS: 0.25–15.07 ng/L (19/19)</lod"). 	orted [43] [11]			
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Drinking water ¹⁶ Spain 2015 PFOS: 2.0–140 ng/L (11/29) [45] Netherlands 2016 PFBS: 0.54–19.0 ng/L (6/6) PFHS: 0.02–0.43 ng/L (6/6) PFHS: 0.02–0.31 ng/L (3/6) [43] Drinking water FFBS: 0.02–0.43 ng/L (14/226) PFOS: <0.03–0.41 ng/L (5/6) [61] Drinking water Canada 2012–2016 PFBS: <1–8.3 ng/L (14/226) PFOS: <0.03–0.41 ng/L (24/25) PFOS: <0.03–0.11 ng/L (24/25) PFOS: <0.03–0.11 ng/L (24/25) [46] Drinking water North America, 2013–2015 PFBS: <0.032–11.1 ng/L (24/25) PFOS: <0.034–44.8 ng/L (23/25) PFOS: <0.034–44.8 ng/L (23/25) PFOS: <0.034–0.44.8 ng/L (23/25) PFOS: <0.034–0.11 ng/L (24/25) [46] DwTP effluent PFBS: <0.032–11.9 ng/L (24/25) PFDS: <0.049 ng/L (0/25) [46] warface water one sediment North America 2010 & 2010 & 2010 & 2010 & 2010 PFBS: <0.032–11.9 ng/L (24/25) PFOS: <0.01–0.048 ng/g dw (27/26) [41] warface water one warface water North America 2010 PFBSA: 0.035–1.99 ng/g dw (27/26) [41] warface water One warface water Soil SpFSAs: 0.037–0.421 ng/g dw (3/3) [47] Asia 2016 2PFSAs: ND–0.144 ng/g dw (4/5) Asia 2016 2PFSAs: 0.026–0.048 ng/g dw (3/3) [47]					
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Image: Section of the secti			Netherlands 2016	PFBS: 0.54–19.0 ng/L (6/6) PFHxS: 0.02–0.43 ng/L (6/6)	[43]
$ \begin{array}{ c c c c c } \hline PFOS: <0.03-0.41 \ ng/L (3/6) \\ \hline \\ $				PFHpS: <0.02–0.03 ng/L (3/6)	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$			Canada 2012–2016	PFOS: <0.03–0.41 ng/L (5/6) PFBS: <1–8.3 ng/L (14/226) PFHxS: <1–2.6 ng/L (43/226) PFOS: <0.5–5.9 ng/L (113/226) PFOS: <0.5–5.9 ng/L (113/226)	[61]
DWTP effluent PFBS: <0.032-11.9 ng/L (24/25) [46] air PFNS: <0.034-21.1 ng/L (20/25)	Drinking water treatment plant (DWTP) influent		North America, 2013–2015	PFDS: <1 ng/L (0/226) PFBS: <0.032–11.1 ng/L (24/25) PFHxS: <0.034–44.8 ng/L (23/25) PFOS: <0.13–48.3 ng/L (22/25) PFDS: <0.049 ng/L (0/25)	[46]
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air surface water \boxtimes soil sedimentone multipleNorth America 2016 $\sum PFSAs: 0.035-1.99 \text{ ng/g dw}}{(33/33)}$ [47]Europe 2016 $\sum 2016$ $\sum PFSAs: ND-3.27 \text{ ng/g dw}}{(9/10)}$ [47]Asia 2016 $\sum PFSAs: ND-3.27 \text{ ng/g dw}}{(6/6)}$ [47]Asia 2016 $\sum PFSAs: 0.079-0.421 \text{ ng/g dw}}{(6/6)}$ [47]Australia 2016 $\sum PFSAs: 0.079-0.421 \text{ ng/g dw}}{(4/4)}$ [47]	☐ air ☐ surface water ☐ soil ⊠ sediment	☐ one ⊠ multiple	Korea 2010 & 2012	PFHxS: ND-0.01 ng/g dw (9/27) PFOS: 0.01-0.048 ng/g dw (27/26)	[11]
Europe Σ PFSAs: ND-3.27 ng/g dw (9/10) 2016 Σ PFSAs: 0.079-0.421 ng/g dw Asia 2016 Σ PFSAs: 0.079-0.421 ng/g dw Africa 2016 Σ PFSAs: ND-0.144 ng/g dw (4/5) Australia Σ PFSAs: 0.044-0.297 ng/g dw 2016 South South Σ PFSAs: 0.026-0.048 ng/g dw (3/3) (3/3)	\square air \square surface water \boxtimes soil	☐ one ⊠ multiple	North America 2016	∑PFSAs: 0.035–1.99 ng/g dw (33/33)	[47]
Asia 2016 ΣPFSAs: 0.079–0.421 ng/g dw (6/6) Africa 2016 ΣPFSAs: ND–0.144 ng/g dw (4/5) Australia ΣPFSAs: 0.044–0.297 ng/g dw 2016 (4/4) South ΣPFSAs: 0.026–0.048 ng/g dw America (3/3)			Europe 2016	\sum PFSAs: ND-3.27 ng/g dw (9/10)	
Africa 2016 ΣPFSAs: ND-0.144 ng/g dw (4/5) Australia ΣPFSAs: 0.044-0.297 ng/g dw 2016 (4/4) South ΣPFSAs: 0.026-0.048 ng/g dw America 2016			Asia 2016	∑PFSAs: 0.079–0.421 ng/g dw (6/6)	
Australia 2016 \sum PFSAs: 0.044–0.297 ng/g dw (4/4) South America 2016 \sum PFSAs: 0.026–0.048 ng/g dw (3/3)			Africa 2016	Σ PFSAs: ND-0.144 ng/g dw (4/5)	
South $\sum_{\text{America}} \text{PFSAs: } 0.026-0.048 \text{ ng/g dw}$ 2016 (3/3)			Australia 2016	∑PFSAs: 0.044–0.297 ng/g dw (4/4)	
			South America 2016	∑PFSAs: 0.026–0.048 ng/g dw (3/3)	

¹⁶ U.S. EPA has also collected nationwide drinking water data for certain PFAS, a summary of which can be found here: <u>https://www.epa.gov/sites/production/files/2017-02/documents/ucmr3-data-summary-january-2017.pdf</u>. Such data were further analyzed in, e.g., Guelfo, J.L. and D.T. Adamson. 2018. Evaluation of a national data set for insights into sources, composition, and concentrations of per- and polyfluoroalkyl substances (PFASs) in U.S. drinking water. *Environmental Pollution* 236 (May): 505–513. Additionally, many U.S. states have also published data on the occurrence of PFAS in drinking water on their websites. Such data were recently analyzed in Andrews, D.Q. and Naidenko, O.V. 2020. Population-wide exposure to per- and polyfluoroalkyl substances from drinking water in the United States. *Environmental Science & Technology Letters* 7(12): 931–936.

Remote regions	☐ air ☐ surface water ⊠ soil ☐ sediment	one Multiple	Antarctica 2016	∑PFSAs: 0.007 ng/g dw (1/1)	[47]
WWTP	⊠ effluent □ sludge	☐ one ⊠ multiple	Germany 2007	PFBS: 1.8–25.9 ng/L (9/9) PFHxS: 0.3–6.3 ng/L (9/9) PFHpS: <0.08–0.5 ng/L (3/9) PFOS: <0.06–82.2 ng/L (7/9) PFOSI: 0.1–1.2 ng/L (9/9)	[44]
	effluent sludge	☐ one ⊠ multiple	United States 2012 & 2013	PFBS: ND-14.0 ng/L (23/28) PFHxS: ND-2.48 ng/L (25/28) PFOS: 2.18-94.4 ng/L (28/28)	[62]
Landfill leachate and impacted groundwater (<i>historic</i> , <i>i.e.</i> <i>closed</i> 25–90 <i>years</i>)		☐ one ⊠ multiple	Canada, 2018	PFBS: NR–710 ng/L (NR) PFHxS: NR–1300 ng/L (NR) PFOS: NR–2800 ng/L (NR) PFDS: NR–2 ng/L (NR) FOSA: NR–13 ng/L (NR) PFECHS: NR–9500 ng/L (NR)	[63]
Indoor environment	Indoor air (hotel rooms) Indoor air (residential homes)	⊠ one □ multiple	China 2015	∑PFSA: 0.0712–0.231 ng/m ³ (13/13) ∑PFSA: 0.0868–0.567 pg/m ³ (19/19)	[48]
	Indoor dust (hotel rooms)			∑PFSA: 2.44–99.1 ng/g (13/13)	
	Indoor dust (residential homes)			∑PFSA: 3.43–72.5 ng/g (19/19)	
Wildlife	Plankton	\square one \square multiple	Korea	PFOS: ND-12.67 ng/g ww (6/12)	[11]
	Crucian carp, blood		2010 & 2012	PFHxS: ND-4.96 ng/ml (26/69) PFOS: 0.18-145.23 ng/ml (69/69) PFDS: ND-0.60 ng/ml (1/69)	[11]
	Crucian carp, liver			PFHxS: ND-0.30 ng/g ww (4/69) PFOS: ND-43.76 ng/g ww (58/69) PFDS: ND-0.58 ng/g ww (9/69)	[11]
	Harbor seals (<i>Phoca vitulina</i> , liver)		Germany 2007	PFBS: ND-0.78 ng/g ww (NR) PFPeS: 0.13-5.38 ng/g ww (NR) PFHxS: 1.11-10.4 ng/g ww (NR) PFHpS: ND-5.43 ng/g ww (NR)	[49]
			1		
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				PFOS: 559–1665 ng/g ww (NR)	
				PFNS: 0.12–1.80 ng/g ww (NR)	
				PFDS: 0.11–1.02 ng/g ww (NR)	
				PFOSI: ND-0.16 ng/g ww (NR)	
	Eggs of Northern Fulmars and Thick-Billed Murres		North America, 2010-2011	PFBS: <0.1–0.57 ng/g ww (range of means, NR/60) PFHxS: <0.1–0.13 ng/g ww (range of means, NR/60) PFOS: <19.8–27.4 ng/g ww (range of means, NR/60) PFDS: <0.2 ng/g ww (NR/60)	[50]
	Ringed seals (Pusa hispida) plasma		Northern Europe, 2010	PFBS: <0.07 ng/g ww (mean, NR/11) PFHxS: 1.29 ng/g ww (mean	[51]
				NR/11)	
				PFOS: 48 ng/g ww (mean, NR/11)	
				PFDS: <0.07 ng/g ww (mean, NR/11)	
	Peregrine falcons, plasma		Canada, 2016 &	PFEtCHxS: ND-3.96 ng/g ww (36/57)	[64]
			2018	PFBS: ND-3.47 ng/g ww (27/57)	
				PFHxS: ND-4.89 ng/g ww (56/57)	
				PFOS: 4.97–124 ng/g ww (57/57)	
	Deregrine	-	Canada	PFDS: ND-8.31 ng/g ww (53/57)	
	falcons, egg		2018	PFEtCHxS: ND–0.26 ng/g ww (7/9)	
				PFBS: ND-0.10 ng/g ww (3/9)	
				PFHxS: 0.09–0.92 ng/g ww (9/9)	
				PFOS: 11.8–53.2 ng/g ww $(9/9)$ PFDS: 0.90–2.63 ng/g ww $(9/9)$	
Human serum	general	-	North	PFHxS: 1 18 ng/ml (mean:	[65]
	population		America,	NR/1993)	
	exposure		2013-2010	PFOS: 4.72 ng/ml (mean; NR/1993)	
	Children age 3–		North	PFBS: <0.07-0.17 ng/ml (27/639)	[52]
	11		2013–2014	PFHxS: <0.07–12.9 ng/ml (638/639)	
				PFOS (linear): <0.07–26.54 ng/ml (639/639)	
				PFOS (branched): <0.07–10.68 ng/ml (639/639)	
	general]	Canada,	PFHxS: 0.9 ng/ml (mean;	[66]
	population		2016-2017		

FACT CARDS OF MAJOR GROUPS OF PER- AND POLYFLUOROALKYL SUBSTANCES (PFASS)

	occupationa			2587/2595)	
	exposure			PFOS: 3.0 ng/ml (mean; 2591/2594)	
Know	vledge gaps				-
- Ver	y little is known about the u	ise, occurrence, a	nd environme	ntal fate of PFSIAs.	
- Curr	rent production volumes ar	e only available a	s estimates.		
- Mor PFHx	re information on PFHxS S risk profile under the Sto	and PFBS can be ckholm Convent	e found in the ion [13], [41],	ir EU REACH SVHC dossiers an [42], [19].	d in the
Refer	ences				
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4. Per- and polyfluoroalkylether carboxylic (a) and sulfonic (b) acids

Key publication: Wang, Zhanyun, Ian T. Cousins, Martin Scheringer, and Konrad Hungerbuehler. 2015. "Hazard Assessment of Fluorinated Alternatives to Long-Chain Perfluoroalkyl Acids (PFAAs) and Their Precursors: Status Quo, Ongoing Challenges and Possible Solutions." *Environment International* 75: 172–79. https://doi.org/10.1016/j.envint.2014.11.013.

Chemical Information & Properties						
Identification and Te	erminology					
Name	Per- and polyfluoroether carboxylic acids	Per- and polyfluoroether sulfonic acids				
Acronym	PFECAs	PFESAs				
Exemplary Chemical Formula	C _n F _{2n+1} OC _m F _{2m} COOH	$C_nF_{2n+1}OC_mF_{2m}SO_3H$				
Exemplary Structure (perfluorinated ones and linear isomers)	$F \xrightarrow{F}_{n} O \xrightarrow{F}_{m} O \xrightarrow{F}_{m} O \xrightarrow{O}_{H}$	$F = \begin{bmatrix} F & F & O \\ C & J & O \\ F & F & F & O \\ F & F & F & O \\ F & F & F & O \\ \end{bmatrix} = OH$				
US EPA CompTox Markush ID	DTXSID001024687	DTXSID301024686				
Degradability, Mobility, Bioconcentration						
Abiotic degradation	Resistant to photolysis, hydrolysis, and OH radical-mediated reactions, under environmentally relevant conditions. [1]	Resistant to photolysis, hydrolysis, and OH radical-mediated reactions, under environmentally relevant conditions [1] F-53B shows only very low degradation in advanced oxidation processes [2]				
Biodegradation	Resistant to biodegradation [1] Not being removed in conventional drinking water treatment plants [3]	Resistant to biodegradation [1] F-53B is not readily biodegradable in closed bottle tests [2]				
Adsorption on PAC	PFECAs have a lower affinity for PAC than other PFASs of similar chain length. About 35% removal of HFPO-DA (CAS Number 62037-80- 3) after 1h with 100 mg/L PAC. [3]					
Bioaccumulation potential	Likely low bioaccumulation potential, with BCF (fish) <10 [4].	$\frac{\text{log BAF}_{\text{frogs, whole body}} (L/kg) = ~3 (6:2 \text{ Cl-PFESA}^{17}) / ~4.2 (8:2 \text{ Cl-PFESA})}{\text{PFESA}^{17}}$				
	Log BAF _{frogs, whole body} (L/kg) = -0.12 (HFPO-TA) [5] $t_{1/2}$ (rats) = 44 h (ADONA)	Black-spotted frogs sampled from several Chinese cities, which have large-scale fluorochemical industries [5]				

 $^{^{17}}$ Note on nomenclature: n:m here refers to the length of the carbon chain on each side of the ether bond. e.g. 6:2 means C₆F₁₃OC₂F₄-. Note that this commonly used nomenclature differs from the nomenclature of n:2 fluorotelomers.

	$t_{1/2}$ (humans) = 23 ± 11 d (ADONA) [1], [6]					
Environmental transport	expected to have similar transport properties as PFCAs [1]					
Synthesis						
Main synthesis method(s)	Some PFECAs are synthesized by an addition reaction of perfluoroalkyl fluorides with hexafluoropropylene oxide (HFPO), catalyzed by alkali-metal fluorides. Subsequent hydrolysis then yields the carboxylic acid. Other synthesis routes, including electrochemical or direct fluorination may exist as well. [7], [8] $F-R_f-C_F^{O}$ + F_F $F_F^{CF_3}$ $\xrightarrow{\text{catalyzed by}}_{\text{alkali-metal fluorides}}$ $F_F^{R_f}C_F_3$ $F_F^{R_f}C_F_3$ $F_F^{R_f}C_F_3$ $F_F^{R_f}C_F_3$ $F_F^{R_f}C_F_3$ $F_F^{R_f}C_F_3$					
Industrial Practices	& Commercial Uses					
Major Commercial I	Products					
Trade name	GenX ¹⁸					
Full name	Hexafluoropropylene oxide-dimer acid, ammonium salt					
Other names	PFPrOPrA, HFPO-DA (acid form) [9]					
Composition	$\overline{CF_3CF_2CF_2OCF(CF_3)COO^- NH_4^+ [10]}$					
CAS Number	62037-80-3					
Production/Import volumes	Registered in 2011 under REACH with a production volume of 10–100 tonnes/yr in the EU. [10]					
Use	Used as a processing aid in fluoropolymer production, replacing APFO. [11]					
Trade name	ADONA					
Full name	3H-Perfluoro-3-[(3-methoxy-propoxy)propanoic acid], ammonium salt					
Composition	$CF_3OC_3F_6OCHFCF_2COO^- NH_4^+$ [6]					
CAS Number	958445-44-8					
Production/Import volumes	Registered under REACH with 1–10 tonnes/yr of production or import in the EU. [12]					
Use	As a processing aid, specifically as emulsifier, in fluoropolymer production. [6]					
Trade name	F-DIOX ammonium salt; cC6O4 ammonium salt					
Full name	Perfluoro{acetic acid, 2-[(5-methoxy-1,3-dioxolan-4-yl)oxy]}, ammonium salt					
Composition	$C_6F_9O_6^-NH_4^+$ [13]					
CAS Number	1190931-27-1					
Production/Import	Registered under REACH with 1–10 tonnes/yr of production or import in the EU. [14]					

¹⁸ Note that GenX has often been used interchangeably with hexafluoropropylene oxide dimer acid (HFPO-DA) and HFPO-DA ammonium salt.

volumes										
Use		As a processing aid in fluoropolymer production. [13]								
Trade name		F-53B								
Composition		ClF ₂ C(CF ₂) ₅ C	$ClF_2C(CF_2)_5O(CF_2)_2SO_3^-K^+[2]$							
CAS Number		73606-19-6								
Use		A mist suppre	essant in chromo	e plating, used	as a substitute to PFOS [2]					
Uses										
Major applicatio	ons	A number of fluoropolyme used as PFOS	A number of PFECAs (usually in the form of their ammonium salts) are used as luoropolymer processing aids, to replace APFO and APFN. [15] PFESAs like F-53B are used as PFOS substitutes, e.g. as mist suppressants in chrome plating [2].							
Regulatory Stat	us									
US		US EPA has r [16]	eleased a draft 1	reference dose	of 80 ng/kg bw per day of HFPO-DA i	in 2018.				
Europe		HFPO-DA ha to its very hig [4]	s been added to h persistence, n	o the list of Sub nobility, and po	bstances of Very High Concern (SVF otential harm to humans and the enviro	IC) due onment.				
Examples of re	port	ed occurrence	S							
Type of	(En	viron-	Detected in	Examples						
locations/ samples	mei	ntal) media	one or multiple regions	Location, year	Levels [min.–max. (detection frequency)]	Ref.				
Note: Non-detect pg = picograms,	ts are ng =	reported as be nanograms, w	low the value o w = wet weight	f the limit of de , ND = not det	etection (" <lod"). ected, NR = not reported</lod"). 					
Close to fluorochemical manufacturing		air surface water soil	☐ one ⊠ multiple	Netherlands 2016	HFPO-DA: 1.7–433 ng/L (13/13)	[7]				
рагк	sediment sediment			US 2013	HFPO-DA: 55–4560 ng/L (34/34)	[3]				
Not close to specific point sources		air surface water soil	□ one ⊠ multiple	Germany & Netherlands 2013	HFPO-DA: <0.11–86.1 ng/L (4/23)	[17]				
		sediment	China 2014	HFPO-DA: <0.25–3060 ng/L (22/29)	[17]					
				China 2013	F-53B: 11.7–54.7 ng/L (7/7)	[2]				
				China 2016	HFPO-DA: <0.05–1.54 ng/L (33/35)	[18]				
					HFPO-TA: <0.1–1.29 ng/L (27/35)					
					4:2 Cl-PFESA: <0.01–0.04 ng/L (4/35)					

				6:2 Cl-PFESA: 0.12–12.94 ng/L (35/35)		
				8:2 Cl-PFESA: <0.01–0.29 ng/L (18/35)	-	
				6:2 H-PFESA: 0.02–4.07 ng/L (35/35)		
			UK	HFPO-DA: 0.7–1.58 ng/L (6/6)	[18]	
			2016	HFPO-TA: <0.1-0.21 ng/L (4/6)		
				6:2 Cl-PFESA: 0.01–0.08 ng/L (6/6)		
			Germany 2016	HFPO-DA: 0.59–1.98 ng/L (20/20)	[18]	
				HFPO-TA: <0.1–0.31 ng/L (14/20)		
				ADONA: <0.01–1.55 ng/L (15/20)		
				6:2 Cl-PFESA: 0.02–0.38 ng/L (20/20)		
			US 2016	HFPO-DA: 0.78–8.75 ng/L (12/12)	[18]	
				HFPO-TA: <0.1–4.33 ng/L (9/12)		
				6:2 Cl-PFESA: <0.01–0.08 ng/L (8/12)		
	Drinking water	☐ one ⊠ multiple	Netherlands 2016	HFPO-DA: <0.2–11 ng/L (3/6)	[7]	
WWTP	☐ effluent☑ influent☑ sludge	☐ one ⊠ multiple	China 2013	F-53B: 79.9–108.7 ng/L (5/5)	[2]	
	 effluent influent sludge 			F-53B: 45.7–74.8 ng/L (5/5)		
Wildlife	Black-spotted frogs (P.	☐ one ⊠ multiple	China	HFPO-TA: <0.05–27.3 ng/g ww (4/56)	[5]	
	<i>nigromaculatus,</i> liver)			6:2 Cl-PFESA: 0.13–119.05 ng/g ww (56/56)		
				8:2 Cl-PFESA: 0.01–14.89 ng/g ww (56/56)		
	Polar bear (liver)		Greenland 2012–2013	F-53B: 0.27 ng/g (mean) (8/8) ¹⁹	[19]	

¹⁹ F-53B was also among a number of halogenated contaminants found in polar bears in Canada between 1984 and 2014 [20].

Knowledge gaps

- Main synthesis pathways for the commercial products of PFECAs and PFESAs.

- Global production volumes of commercial PFECAs and PFESAs.

- More information on the bioaccumulation potential needed.

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5. Perfluoroalkanoyl fluorides (a) and their derivatives (b)²⁰

Chemical Informati	ion & Properties	
Identification and Te	erminology	
Name	Perfluoroalkanoyl fluorides	Perfluoroalkyl fluoride derivatives
Acronym	PACFs	PACF-based derivatives
Chemical Formula	$C_{n-1}F_{2n-1}COF$	$C_{n-1}F_{2n-1}CONR_2$ (e.g. perfluoroalkyl amides, PFAMs) ²¹
General Structure (linear isomers)	$F = \begin{bmatrix} F \\ C \\ B \end{bmatrix}_{n-1} \begin{bmatrix} 0 \\ C \\ F \end{bmatrix}$	$F = \begin{bmatrix} F \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\$
US EPA CompTox Markush ID	DTXSID10893647	
Examples of Individual Acronyms (as used in this document)		MeFOA: $n = 8$, $R^1 = CH_3$, $R^2 = H$ EtFOA: $n = 8$, $R^1 = CH_2CH_3$, $R^2 = H$ EtFBA: $n = 4$, $R^1 = CH_2CH_3$, $R^2 = H$
Degradability, Mobil	lity, Bioconcentration	
Degradation	PACFs hydrolyze when released into the environment and form the corresponding perfluoroalkyl carboxylic acids (PFCAs), similarly to PASFs [1], [2]. These PFCAs then are persistent in the environment; for more information, see the fact card #2 on perfluoroalkyl carboxylic acids and perfluoroalkyl dicarboxylic acids.	MeFOA and EtFOA are expected to volatilize to the atmosphere and react with hydroxyl radicals, ultimately forming perfluorinated carboxylic acids (PFCAs) [2]. EtFBA is shown to degrade to PFBA, PFPrA, and TFA, among other products. [3]
Atmospheric lifetime		MeFOA: approx. 19 days (estimate) EtFOA: approx. 2.7 days (estimate) EtFBA: approx. 4.4 days (estimate) Perfluorobutyramide (the primary oxidation product of EtFBA): 7 times EtFBA [3]
Synthesis		
Main Synthesis Method	Electrochemical fluorination of an alkanoyl $C_n H_{2n+1}COF + (2n+1)HF -$	fluoride [1] $\rightarrow C_n F_{2n+1} COF + (2n+1)H_2$

²⁰ For more examples of compounds in this group and their associated information, one may search for the following IDs at the U.S. EPA CompTox Chemicals Dashboard website: <u>https://comptox.epa.gov/dashboard</u>, namely DTXSID10893647, DTXSID70893648, DTXSID50893883, DTXSID10893884, DTXSID70893885, DTXSID30893886, DTXSID90893887, DTXSID10893889, DTXSID20893890, DTXSID80896827

²¹ Note that PFCAs are also considered PACF-derivatives, but are discussed in their own fact card #2.

	Reaction of these PACFs or of perfluoroalkanoyl chlorides with amines yields PFAMs:
	$C_n F_{2n+1} COF + NH_2 R \longrightarrow C_n F_{2n+1} CONHR + HF$
	PFAMs are also produced as by-products from POSF-based syntheses [2].
Possible Impurities	The electrochemical fluorination process is unselective and yields, besides the target compound, a mixture of linear, branched, and cyclic homologues, which can be found as impurities in the final product [1], [4].
Industrial Practices	& Commercial Uses
Major Commercial I	Products
Full name	Perfluorobutanoyl fluoride (PBCF)
Composition	C ₃ F ₇ COF
CAS Number	335-42-2
Production/Import volumes	500 - <10,000t in the US in 2015 [11].
Use	Production of PFBA and potentially other, unknown uses [5].
Full name	Perfluorooctanoyl fluoride (POCF, sometimes also PFOF)
Composition	C ₇ F ₁₅ COF
CAS Number	335-66-0
Production/Import volumes	0 lbs in the US in 2015 [11].
Use	Used to produce PFOA [1], [6].
Full name	N-(3-Trimethoxysilylpropyl)perfluorohexanamide
Composition	$CF_3(CF_2)_4CONH(CH_2)_3Si(OCH_3)_3$
CAS Number	154380-34-4
Use	Surface treatment of glasses, natural stones, metals, wood, cellulose, cotton, leather, and ceramics [5]. ²²
Uses	
Major applications	PACFs are raw materials or intermediates in the production of the respective carboxylic acids and derivatives thereof [5]. For example, POF is an intermediate in the production of PFOA [1], [6].
Regulatory Status	
General remarks	Since PACFs and their derivatives are precursors to PFCAs, most regulatory activities are directed towards PFCAs, but include PACFs explicitly or implicitly.
US	Under the 2010/2015 PFOA Stewardship Program by the US EPA, eight major multinational fluoropolymer and fluorotelomer PFCA manufacturers started to phase out long-chain PFCAs in 2006, which was achieved by 2015. [4] In July 2020, the US EPA issued a final rule requiring notice and US EPA review before manufacturing/processing

 $^{^{22}}$ Note that these might be historical uses, as the manufacturer, Miteni, has declared bankruptcy since 2018 [10].

	of certain long-chain PFASs that have been phased out in the United States could commence. [7]
Europe	PFOA and its ammonium salt (APFO), as well as some related substances, including POF, have been classified as substances of very high concern (SVHCs) under REACH in 2013. In 2017, these substances were also added to the restricted substances list. [4]

International efforts

PFOA, its salts and PFOA-related compounds are listed as POPs (persistent organic pollutants) under Annex A (Elimination) to the Stockholm Convention with several specific exemptions (see listing for the chemical definition of PFOA-related compounds covered) [8].

PFOA, its salts and PFOA-related compounds are recommended by the Chemical Review Committee (CRC) of the Rotterdam Convention for listing under the Convention (to be determined by the Conference of the Parties (COP) in 2022). [9]

Examples of reported occurrences

Note: As noted above, PACFs and their derivatives form the corresponding carboxylic acids when released to the environment, similarly to PASFs. For examples of reported occurrences of the carboxylic acids in the environment, see the fact card #2 on PFCAs and PFdiCAs. No direct measurements of PACFs or their derivatives (other than PFCAs) in the environment have been found.

Knowledge gaps

- Information on recent uses and production volumes of PACFs is very limited.

- Information on PACF-based derivatives (such as PFAMs) is very limited and no environmental monitoring studies of these compounds could be found.

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ENV/CBC/MONO(2022)1 | 51

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6. Perfluoroalkanesulfonyl fluorides (a) and their derivatives (b) ²³

Chemical Information & Properties			
Identification and Te	erminology		
Name	Perfluoroalkanesulfonyl fluorides	Perfluoroalkanesulfonyl fluoride derivatives	
Acronym	PASFs	PASF-based derivatives	
Chemical Formula	$C_nF_{2n+1}SO_2F$	$C_n F_{2n+1} SO_2 NR_2$ (example of a sulfonamide)	
General Structure (linear isomers)	$F = \begin{bmatrix} F & O \\ C & S \end{bmatrix} = F$ $F = \begin{bmatrix} C & S \\ C & S \end{bmatrix} = F$ $F = O$	$F = \begin{bmatrix} F \\ C \\ F \\ F \\ F \\ F \\ F \\ F \\ C \\ F \\ C \\ R \\ (example of a sulfonamide)$	
US EPA CompTox Markush ID	DTXSID601024685	DTXSID501024694	
Examples of Individual Acronyms (as used in this document)	POSF: n = 8	FOSA: n = 8, R = H MeFOSA: n = 8, R ¹ = CH ₃ , R ² = H MeFOSE: n = 8, R ¹ = CH ₃ , R ² = CH ₂ CH ₂ OH EtFOSA: n = 8, R ¹ = CH ₂ CH ₃ , R ² = H EtFOSE: n = 8, R ¹ = CH ₂ CH ₃ , R ² = CH ₂ CH ₂ OH MeFBSA: n = 4, R ¹ = CH ₃ , R ² = H MeFBSE: n = 4, R ¹ = CH ₃ , R ² = CH ₂ CH ₂ OH SAmPAP diester: <i>N</i> -ethyl perfluorooctane sulfonamido ethanol-based phosphate diester	
Degradability, Mobi	lity, Bioconcentration	-	
Degradation	PASFs rapidly hydrolyze to form the corresponding sulfonic acids [1]. These sulfonic acids then are persistent in the environment, for more information see the fact card #3 on perfluoroalkane sulfonic and sulfinic acids.	Biotic degradation of perfluorosulfonamides mostly yields the corresponding sulfonic acids ²⁴ , while abiotic degradation yields sulfonic acids, carboxylic acids, and other degradation products [2] [3]. For example, EtFOSE is transformed in marine sediments to <i>N</i> -ethyl perfluorooctane sulfonamidoacetate, perfluorooctane	

²³ For more examples of compounds in this group and their associated information, one may search for the following IDs at the U.S. EPA CompTox Chemicals Dashboard website: https://comptox.epa.gov/dashboard, namely DTXSID50892977, DTXSID10892978, DTXSID80893634, DTXSID40893635, DTXSID70896775, DTXSID30896832, DTXSID101010201, DTXSID801010202, DTXSID701010209, DTXSID701010211, DTXSID101010213, DTXSID001010234, DTXSID701010235, DTXSID401010236, DTXSID101010237, DTXSID801010238, DTXSID501010239, DTXSID801010240, DTXSID501010241, DTXSID201010242, DTXSID901010243, DTXSID601010244, DTXSID201010254, DTXSID901010255, DTXSID601010256, DTXSID301010257, DTXSID001010258, DTXSID701010259, DTXSID001010260, DTXSID701010261, DTXSID401010262, DTXSID101010263

 $^{^{24}}$ For more information on those compounds, see the fact card #3 on perfluoroalkane sulfonic and sulfinic acids.

		sulfonamidoacetate, <i>N</i> -ethyl perfluorooctane sulfonamide, perfluorooctane sulfonamide, and perfluorooctane sulfonate, with $t_{1/2}$ =44 d (25°C) and 160 d (4°C). SAmPAP diester showed little to no biotransformation over 120 d. [4]	
Adsorption on soil & sediment		FOSA adsorbs strongly to organic matter, making soils an important environmental sink [5].	
Bioaccumulation potential		FOSA can be accumulated by various plants [5].	
Synthesis	<u>.</u>		
Main Synthesis Method	Mostly the Simons electrochemical fluorination process is used, where the hydrocarbon sulfonyl fluoride is electrolyzed in anhydrous hydrogen fluoride [6]:		
	$C_n H_{2n+1} SO_2 F + (2n+1) I$	$HF \longrightarrow C_n F_{2n+1} SO_2 F + (2n+1)H_2$	
	Reaction with an amine then yields sub $C_n F_{2n+1} SO_2 F + RNF_2$	fonamides: $H_2 \longrightarrow C_n F_{2n+1} SO_2 NHR + HF$	
	These can be further reacted with, for example, ethylene carbonate, to give perfluoroalkane sulfonamido ethanols. Possible subsequent reaction steps can yield <i>N</i> -alkyl perfluoroalkane sulfonamidoethyl acrylates and <i>N</i> -alkyl perfluoroalkane sulfonamidoethyl methacrylates. [1]		
Possible Impurities	The electrochemical fluorination process is unselective and yields, besides the target compound, a mixture of linear, branched, and cyclic homologues, which can be found as impurities in the final products [1], [7].		
Industrial Practices	& Commercial Uses		
Major Commercial I	Products		
Full name	Perfluorooctane sulfonyl fluoride (POS	5F)	
Composition	$C_8F_{17}SO_2F$		
CAS Number	307-35-7		
Production/Import volumes	Globally: 96 000 tonnes (estimated) be and 2008 [8]	tween 1970 and 2002; 410 tonnes between 2003	
	China: 250 tonnes (estimated) between	2003 and 2008 [8]	
	Japan: 100 tonnes between 2003 and 20 Germany: 25 tonnes between 2003 and	008 [8]	
Full name	Perfluorobutane sulfonyl fluoride (PRS	2006 [6]	
Composition	C4FoSO2F	/* /	
CAS Number	375-72-4		
Production/Import volumes	Global production: in total, 317 tonnes	in 2015 (299 tonnes in China). [9]	
Full name	Sulfluramid / N-ethyl perfluorooctane	sulfonamide	
Composition	$C_8F_{17}SO_2NH(C_2H_5)$		

CAS Number	4151-50-2
Production/Import	Production phased out in the US. [1], [10]
volumes	Production in Brazil in 2013 was estimated to be about 60 tonnes. [10]
Uses	Pesticide, especially used against leaf-cutter ants [1] [10]
Full name	Sodium 2-(<i>N</i> -ethylperfluorooctane-1-sulfonamido)ethyl phosphate / perfluorooctane sulfonamido ethanol-based phosphate diester / SAmPAP
Composition	$F_3C(F_2C)_7SO_2N(C_2H_5)CH_2CH_2OPO(ONa)_2$
Production/Import volumes	A high production volume chemical until 2002, then phased out in North America. [4]
Uses	Used in food contact paper and packaging until it was phased out in North America 2002 [4]
Other PASF derivatives	PBSF-derivatives are used as surfactants (e.g. in coatings), as intermediates in the manufacture of other chemicals, or as plastic additives. [9] Other PASF derivatives, such as <i>N</i> -MeFOSEA and <i>N</i> -EtFOSE, have been produced by
	3M (which were phased out in 2002) and others [1]. They were used in surface treatment products, as paper protectors, and as performance chemicals (e.g. fire extinguishing foams and surfactants) [11].
Uses	
Major applications	PASFs are used as starting material in the synthesis of sulfonamides and other derivatives including side-chain fluorinated polymers, which have been and are used as plant growth regulators, herbicides, in paper-protecting applications, and as surfactants and surface protection products in other applications [1], [2], [6]. PASFs are precursors to PFSAs with the same chain length [8].
Regulatory Status	
US	In 2002, 3M - the then largest manufacturer of POSF phased out the production of POSF- based products, in agreement with the US EPA [7]. Certain PASFs are subject to a TSCA significant new use rule [12]. US EPA cancelled the last remaining manufacturing-use product registration for Sulfluramid in May 2008 and all remaining pesticide end-use product registrations by 2013. [13]
Canada	Some of these substances are precursors to PFOS, and they were assessed and managed along with PFOS, its salts and precursors in 2006. They are prohibited with a limited number of exemptions under the Prohibition of Certain Toxic Substances Regulations, 2012 [14], [15]
Europe	PFOS and its derivatives (including POSF and FOSA) are regulated as persistent organic pollutants (POPs) and their production, sale, and use in the EU is prohibited, with certain exemptions [8]. PFBS, PFHxS and their salts are listed as SVHC under REACH [16].
International efforts	
POSF ²⁵ was added to	Annex B to the Stockholm Convention as POP in 2009, together with PFOS and its salts.
POSF was added to A sulfonates, perfluoroo	annex III to the Rotterdam Convention in 2013, together with PFOS, perfluorooctane octane sulfonamides. [21]

 $^{^{25}}$ In the Stockholm Convention and the Rotterdam Convention the acronym PFOSF is used.

ENV/CBC/MONO(2022)1 | 55

Examples of reported occurrences					
Type of	(Environmental)	Detected in	Examples		
locations/ samples	media	one or multiple regions	Location, year	Levels [min. –max. (detection frequency; substance)]	Ref.
Note: As noted (not in the case perfluoroalkyl o	above, PASFs and th of PASFs). For exam carboxylic and dicarbo	eir derivatives t ples of reportec oxylic acids and	ransform in the l occurrences of l #3 on perfluo	e environment, forming PFSAs and P of those, see the fact cards #2 on roalkane sulfonic and sulfinic acids.	FCAs
Non-detects are pg = picogram.	e reported as below th s, ng = nanograms, N	e value of the li D = not detecte	imit of detectio ed, NR = not re	n (" <lod"). ported</lod"). 	
Close to WWTP and	air surface water	one 🗌 multiple	Canada 2009	MeFOSA: 6.11–48.2 pg/m ³ (16/16)	[17]
landillis	Soll			EtFOSA: 6.07–30 pg/m ³ (16/16)	
				MeFOSE: 1.06–41.5 pg/m ³ (16/16)	
				EtFOSE: <4.8–29.2 pg/m ³ (16/16)	
Not close to specific point sources	☐ air ⊠ surface water ☐ soil ☐ sediment	☐ one ⊠ multiple	Germany 2007	FOSA: 0.1–1.0 ng/L (15/15)	[18]
WWTP and	effluent	one	Germany	FOSA: 0.3–1.1 ng/L (9/9)	[18]
on-site septic	influent	M multiple	2007	MeFBSA: <0.17–14 ng/L (3/9)	
5				MeFBSE: <0.07–0.5 ng/L (3/9)	
	effluent sludge	☐ one ⊠ multiple	United States 2012 & 2013	PFOSA: ND-6.56 ng/L (12/28)	[22]
Wildlife	Peregrine falcons, serum	⊠ one □ multiple	Canada, 2018	FOSA: ND-0.12 ng/g ww (5/29) MeFOSA: ND-0.05 ng/g ww (3/29) EtFOSA: ND-0.02 ng/g ww (1/29)	[23]
	Peregrine falcons, egg	⊠ one □ multiple	Canada, 2018	FOSA: ND (0/9) MeFOSA: ND (0/9) EtFOSA: ND–0.01 ng/g ww (1/9)	
Knowledge ga	ps				
- Current con volumes), are l	nmercial products of largely unknown.	f PASF-deriva	ntives, especia	ally their production and uses (in	cluding

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7. n:2 Fluorotelomer-based compounds

Key publications: J. W. Washington, T. M. Jenkins, K. Rankin, and J. E. Naile. 2015. Decades-Scale Degradation of Commercial, Side-Chain, Fluorotelomer-Based Polymers in Soils and Water. Environ. Sci. Technol., 49(2): 915–923.

Buck, Robert C, James Franklin, Urs Berger, Jason M Conder, Ian T Cousins, Pim de Voogt, Allan Astrup Jensen, Kurunthachalam Kannan, Scott A Mabury, and Stefan PJ van Leeuwen. 2011. "Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification, and Origins." *Integrated Environmental Assessment and Management* 7 (4): 513–41.

Chemical Information & Properties				
Identification and To	erminology			
Name	n:2 Fluorotelomers	n:2 Fluorotelomer olefins		
Acronym	n:2 FT[R], e.g. FTOH	n:2 FTO		
Chemical Formula	$C_nF_{2n+1}C_2H_4R$	$C_nF_{2n+1}C_2HR^1R^2$		
General Structure (linear isomers)	$F \xrightarrow[F]{} H \xrightarrow[F]{} R^{1}$ $F \xrightarrow[F]{} H \xrightarrow[F]{} R^{2}$ $R^{1} \text{ and } R^{2} = \text{H, unless for carboxylic acids}$	$F \xrightarrow{F}_{n} \xrightarrow{H}_{n} \xrightarrow{R^{1}}_{R^{2}}$		
US EPA CompTox Markush ID	DTXSID401024691	DTXSID601024928		
Terminology	n:m FT[R], where $n =$ number of perfluorinated carbons and $m =$ number of non-fluorinated carbons.			
Overview of n:2 Flue	orotelomer derivatives [1] ²⁶			

²⁶ For more examples of compounds in this group and their associated information, one may search for the following IDs at the US EPA CompTox Chemicals Dashboard website: <u>https://comptox.epa.gov/dashboard</u>, namely DTXSID50892558 (FTSAs), DTXSID90893802 (FTOHs), DTXSID50892972, DTXSID70892974, DTXSID30892975, DTXSID90892976, DTXSID40893817, DTXSID70893820, DTXSID80893876, DTXSID60893879, DTXSID301010245, DTXSID801010264, DTXSID501010265. In addition, fluorinated acrylate and urethane polymers belong to so-called "side-chain fluorinated polymers" (polymers with nonfluorinated polymer backbones and fluorinated side chains).

ENV/CBC/MONO(2022)1 | 59



²⁷ Note that often a different nomenclature is used for FTUCAs in literature. According to this nomenclature,

⁶:2 FTUCA is referred to as F**H**UEA, **8**:2 FTUCA as F**O**UEA, and so forth. This fact card will keep the general n:2 fluorotelomer nomenclature though.

FACT CARDS OF MAJOR GROUPS OF PER- AND POLYFLUOROALKYL SUBSTANCES (PFASS)

	sFTOH (40% _{mol}) after 2 months [10].		
Metabolism in mammals	FTOHs are mostly rapidly eliminated in urine as conjugates, although PFCAs have also been detected as transformation products [3]. In rats, 8:2 FTOH has been found to be excreted mainly via feces, with metabolites including 7:2 sFTOH, 7:2 Ketone, and PFOA, among others [11]. 6:2 FTOH is reported to be rapidly metabolized and eliminated in humans, although its main metabolites PFHxA, PFHpA, PFBA, and 5:3 Acid can exhibit elimination half-lives of 1–2 months after a period of high exposure [12].		
Mobility	FTOHs generally exhibit high volatilities and poor water solubilities, resulting in high water-air partition coefficients and high tendency for sorption onto particles when dissolved in water. [2]		
Synthesis			
Main Synthesis Method	Telomerization: A perfluoroalkyl iodide (usually perfluoroethyl iodide) is reacted with tetrafluoroethylene to increase the perfluorinated chain length. Subsequently, ethylene is inserted (using catalysts or increased temperature and pressure) to form perfluoroalkyl ethyl iodides [3] $E(CE) = E(CE) = E(CE) = E(CE) = E(CE) = E(CE)$		
	$F(CF_2)_n I + CF_2 = CF_2 \longrightarrow F(CF_2)_n CF_2 CF_2 I_2 $		
Possible Impurities	The telomerization process yields only homologues. Whether they are linear (common) or branched (uncommon) isomers, depends on the starting perfluoroalkyl iodide [3].		
Industrial Practices	& Commercial Uses		
Major Commercial H	Products ²⁸		
Full name	6:2 Fluorotelomer sulfonamide betaine		
Composition	$F(CF_2)_6(CH_2)_2SO_2NH(CH_2)_3NH_2^+CH_2COOH$		
CAS Number	34455-29-3		
Production/Import volumes	Registered in the EU under REACH with a production/import volume of 100–1000 t/yr. [13]		
Use	Used in fire-fighting foams, professional cleaning products, and inks and films. [13]		
Full name	Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane		
Composition	$F(CF_2)_6(CH_2)_2Si(OCH_2CH_3)_3$		
CAS Number	51851-37-7		
Production/Import volumes	Registered in the EU under REACH with a production/import volume of 10–100 t/yr. [14]		
Use	Used as oil/water repellence for carpets, fabric/upholstery, apparel, leather and glass. [14]		
Full name	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulfonic acid		
Other names	6:2 Fluorotelomer sulfonic acid		
Composition	F(CF ₂) ₆ (CH ₂) ₂ SO ₃ H		
CAS Number	27619-97-2		
Production/Import volumes	Registered in the EU under REACH with a production/import volume of 10–100 t/yr. [15]		

 $^{^{28}}$ Note that these are just some examples of fluorotelomer-based products, not including polymers. For a more comprehensive overview see the overview figure above.

Use		Used as a mist suppressant in metal plating [15]				
Uses						
Major applicati	ions	Raw material intermediates such as n:2 FTOHs are used to produce surfactants and surface protectors, including side-chain fluorinated polymers. n:2 FTSAs are also directly used as surfactants. diPAPs have also been used as grease-proofing agents for food-contact paper, as defoaming adjuvants in pesticide formulations and as surfactants in industrial cleaning products [3]. For more details on the applications of side-chain fluorinated polymers, see Buck et al. (2011).				
Regulatory Sta	atus					
US		Some of these substances are regulated under 40 CFR §721.10536, the long-chain perfluoroalkyl carboxylate chemical substances significant new use rule. [16] A final rule to revoke tolerance exemptions for mono- and bis- $(1H, 1H, 2H, 2H)$ -perfluoroalkyl) phosphates where the alkyl group is even numbered and in the C ₆ -C ₁₂ range was published in August 2006 with an effective date 18 months after the publication of the final rule. [17] Under the 2010/2015 PFOA Stewardship Program by the US EPA, eight major multinational fluoropolymer and fluorotelomer PFCA manufacturers started to phase out long-				
Canada		Certain fluorotelomers (including diPAPs) are precursors to PFOA and long-chain (C ₉ - C_{20}) PFCAs. Non-exhaustive lists of precursors to PFOA and long-chain (C ₉ - C_{20}) PFCAs can be found in the ecological screening assessments for PFOA and long-chain (C ₉ - C_{20}) PFCAs [18], [19]. These substances are prohibited with a limited number of exemptions under the Brachibitian of Cartain Torio Substances Presultting 2012 [20]			in (C ₉ – PFCAs C ₉ –C ₂₀) der the	
Europe		(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) silanetriol and any of its mono-, di- or tri-O- (alkyl) derivatives (TDFAs) have been added to the restricted substances list (REACH Annex XVII) in 2021. [27]			or tri-O- REACH	
International e	efforts					
Some long-chai Convention on	in fluoi Persist	rotelomers (n≥8 ent Organic Po	8 and n≤16) are llutants. [28]	considered PF	OA-related compounds under the Sto	ckholm
Examples of r	eporte	ed occurrence	S			
Type of	(Env	ironmental)	Detected in	Examples		
locations/ samples	medi	a	one or multiple regions	Location, year	Levels [min.–max. (detection frequency)]	Ref.
Non-detects are pg = picograms	e repor s, ng =	ted as below th nanograms, N	e value of the li D = not detecte	<i>imit of detection</i> d, NR = not re	n (" <lod"). ported</lod"). 	
Close to WWTP and landfills	⊠ ai □ su □ so □ se	r Irface water bil bdiment	☐ one ⊠ multiple	Canada 2009	6:2 FTOH: 0.09–12.3 ng/m ³ (16/16) 8:2 FTOH: 0.14–17.4 ng/m ³ (16/16) 10:2 FTOH: 0.07–2.15 ng/m ³ (16/16)	[10]
	Land	ini leachate		US	4:2 FTUCA: ND–6.3 ng/L (1/87)	[23]

			2013–2014	6:2 FTUCA: <2.0–52.0 ng/L (45/87) 8:2 FTUCA: <2.0–161 ng/L (24/87) 10:2 FTUCA: ND–49.3 ng/L (9/87) 4:2 FTSA: <5.0–22.7 ng/L (22/87) 6:2 FTSA: <2–2247.8 ng/L (84/87) 8:2 FTSA: <2–667.0 ng/L (64/87) 6:2 diPAP: <1.9–26.4 ng/L (14/87) 8:2 diPAP: <2.0–208.8 ng/L (12/87) 10:2 diPAP: ND–47.7 ng/L (6/87)	
Not close to specific point sources	i air Surface water soil sediment	∐ one ⊠ multiple	Germany 2007	6:2 FTSA: <0.2–1.1 ng/L (8/15) 8:2 FTUCA: <0.01–0.1 ng/L (1/15) 10:2 FTUCA: <0.03–0.3 ng/L (3/15)	[21]
			Japan 2007–2008	8:2 FTOH: <0.2–3.38 ng/L (19/33) 10:2 FTOH: <0.2–4.06 ng/L (4/33) 8:2 FTAc: <0.05–0.16 ng/L (6/33)	[22]
WWTP	 effluent influent sludge 	☐ one ⊠ multiple	Germany 2007	6:2 FTOH: <0.2–37.9 ng/L (5/9) 6:2 FTUCA: <0.07–0.9 ng/L (1/9)	[21]
Indoor environment	Indoor air, hotels	i one ⊠ multiple	China 2015	6:2 FTOH: <0.026–1.9 ng/m ³ (16/19) 8:2 FTOH: 0.253–48.0 ng/m ³ (19/19) 10:2 FTOH: 0.054–13.6 ng/m ³ (19/19) 6:2 diPAP: <0.001–0.0067 ng/m ³ (10/19) 8:2 diPAP: <0.002–0.0177 ng/m ³ (6/19) 6:2 FTUCA: <0.002–0.0084 ng/m ³	[24]

				(13/19)	
				8:2 FTUCA: <0.001–0.005 ng/m ³ (13/19)	
	Indoor dust, hotels		China 2015	6:2 FTOH: 4.71–372 ng/g (11/11)	[24]
				8:2 FTOH: 15.6–438 ng/g (11/11)	
				10:2 FTOH: 3.96–123 ng/g (11/11)	
				6:2 diPAP: 1.08–67.4 ng/g (11/11)	
				8:2 diPAP: <0.06–115 ng/g (10/11)	
				6:2 FTUCA: <0.06–0.75 ng/g (6/11)	
				8:2 FTUCA: 0.11–8.29 ng/g (11/11)	
	Indoor dust, residential		Germany 2008–2009	6:2 FTOH: <1.6–246 ng/g (24/31)	[25]
				8:2 FTOH: 2.4–256 ng/g (31/31)	
				10:2 FTOH: 1.0–232 ng/g (31/31)	

Knowledge gaps

- Current global production and use volumes are unknown.

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 [Online]. Available at: <u>https://echa.europa.eu/documents/10162/57497ef0-ee60-a9e9-8bd1-9daba3b3c427</u> [Accessed: 26-May-2021].
- [28] Stockholm Convention on Persistent Organic Pollutants, "Report of the Conference of the Parties to the Stockholm Convention on Persistent Organic Pollutants on the work of its ninth meeting," Geneva, 2019. Decision SC-9/12.

8. n:1 Fluorotelomer-based compounds

Chemical Information & Properties					
Identification and Te	Identification and Terminology				
Name	n:1 Fluorotelomers ²⁹				
Acronym	n:1 FT[R], e.g., n:1 FTOH ³⁰				
Chemical Formula	$C_nF_{2n+1}CH_2OH$				
General Structure (linear isomers)	$ \begin{array}{c} F \\ F \\ F \\ \hline \\ C \\ \hline \\ F \\ \hline \\ F \\ \hline \\ \\ F \\ \hline \\ \\ \\ \\ \\$				
	$R = e.g. OH, NH_2, I$				
US EPA CompTox Markush ID	DTXSID901024684				
Terminology	n:m FT[R], where $n =$ number of perfluorinated carbons and $m =$ number of non-fluorinated carbons				
Degradability, Mobil	lity, Bioconcentration				
Degradation	n:1 FTOHs can react with OH radicals in the environment to form corresponding aldehydes and subsequently carboxylic acids [1].				
Reaction with OH	3:1 FTOH: $1.0-1.1 \times 10^{-13} \text{ k}_{(OH+R)}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$				
radicals	Note: The reaction rate constant is likely largely independent of the chain length, and therefore, valid also for other n:1 FTOHs [1].				
Synthesis					
Main Synthesis Method	n:1 Fluorotelomer compounds are NOT produced via the telomerization process. Instead, they are synthesized through catalytic reduction (hydrogenation) of the corresponding perfluoroalkyl carboxylic acids [1], [2]. For example, LiAlH ₄ can be used to produce n:1 FTOHs [3]: $F(CF_2)_nCOOH \xrightarrow{LiAlH_4} F(CF_2)_nCH_2OH$				
Possible Impurities	Unreacted PFCAs may remain as impurities in n:1 fluorotelomer derivative products. Additionally, the PFCAs themselves, which are used as starting material, are likely to contain both branched and linear isomers, due to them being produced via the ECF process. [1]				
Industrial Practices	& Commercial Uses				
Major Commercial H	Products				

 $^{^{29}}$ As known commercial *n*:1 fluorotelomer-based compounds are not derived from the telomerization process, but rather from the reduction of perfluoroalkyl carboxylic acids, they are not, strictly speaking, fluorotelomers. Despite this, they are termed "n:1 FT-based compounds" here for readability, since the pattern of the perfluorocarbon:hydrocarbon chain is the same (i.e., n:1 vs. n:2). Future work may consider to identify more proper terminology for this group of PFASs. ³⁰ While other n:1 fluorotelomers (such as n:1 fluorotelomer amins or iodides) exist [4], no information on

them could be found.

Trade	Name	RM 610		
Full N	lame	(Perfluoropropyl)methanol (3:1 FTOH)		
Comp	osition	C ₃ F ₇ CH ₂ OH		
CAS I	Number	375-01-9		
Use		Used as monomers to produce side-chain fluorinated polymers. [1]		
Uses				
Major	r applications	<i>tions</i> Acrylates or methacrylates of n:1 FTOHs are monomers used to produce side-chain fluorinated polymers, which can be used as levelling agents, dispersants, and oil and water repellents, especially for textiles and electronics [1], [5].		
Regu	latory Status			
US		Together with the phase-out of other long-chain PFAS and in agreement with the EPA 3M ceased its production of 7:1 FTOH (used to produce acrylate and methacrylat monomer for side-chain fluorinated polymethacrylate-acrylate copolymers – e.g., CA Number 53515-73-4) in 2002. [1]		
Know	vledge gaps			
- Rec	ent production a	and use volumes of n:1 FTOHs and their derivatives are unknown.		
- Kno chain	wledge about t fluorinated acr	he environmental fate of n:1 FTOHs is very limited, especially regarding their side- ylate and methacrylate polymers.		
- Kno	wledge about o	ther n:1 fluorotelomers is very sparse.		
Refer	ences			
[1]	Z. Wang, I. T. Cousins, M. Scheringer, R. C. Buck, and K. Hungerbühler, "Global emission inventories for C ₄ –C ₁₄ perfluoroalkyl carboxylic acid (PFCA) homologues from 1951 to 2030, part II: The remaining pieces of the puzzle," <i>Environ. Int.</i> , vol. 69, pp. 166–176, Aug. 2014.			
[2]	B. Sha, E. L. Schymanski, C. Ruttkies, I. T. Cousins, and Z. Wang, "Exploring open cheminformatics approaches for categorizing per- and polyfluoroalkyl substances (PFASs)," <i>Environ. Sci. Process. Impacts</i> , vol. 21, no. 11, pp. 1835–1851, 2019.			
[3]	D. R. Husted,	and A. H. Ahlbrecht, "Fluorinated alcohols and acetate esters," US 2666797, 1954.		
[4]	OECD, "Ne https://www.o	ew Comprehensive Global Database of PFASs," [Online]. Available: ecd.org/chemicalsafety/portal-perfluorinated-chemicals/ [Accessed: 24-Jul-2020]		
[5]	R. E. Banks, B Applications. 1	E. Smart, and J. C. Tatlow, Eds., Organofluorine Chemistry. Principles and Commercial New York: Springer Science + Business Media, LLC, 1994.		

9. Perfluoroalkylethers (a), epoxides (b), and vinyl ethers (c) (non-polymers)

Chemical Information & Properties				
Identification and Te	erminology			
Name	Perfluoroalkylethers ³¹ Trade names: Fluorinert liquids; galden fluorinated fluids [1]	Perfluoroalkyl epoxides	Perfluorovinyl ethers	
Acronym	PFEs	PFEp	PFVEs	
Chemical Formula (linear isomers)	e.g. $C_nF_{2n+1}OC_mF_{2m+1}$	$C_nF_{2n}OC_mF_{2m}$	RO(C ₃ F ₆ O)CF=CF ₂	
General Structure	$F = F$ $F = C = \int_{n}^{F} O = C = \int_{m}^{F} F$ $F = F$	$F \xrightarrow{F} C \xrightarrow{C} C \xrightarrow{F} C \xrightarrow{F} F$	$R \longrightarrow O \xrightarrow{F}_{F} O \xrightarrow{F}_{R} O \xrightarrow{F}_{F} O F$	
US EPA CompTox Markush ID	DTXSID90893882	DTXSID501024682	DTXSID301024929	
Synthesis		-		
Main Synthesis Method	Electrochemical fluorination of aliphatic ethers, alcohols, or carboxylic acids, or fluorination of ethers with cobalt fluoride or elemental fluorine under controlled conditions [1]		HFPO (hexafluoropropylene oxide) is reacted with a fluorinated alkoxide or other nucleophiles. This yields acid fluorides, which are then converted to acid salts that are subsequently heated in an aprotic environment to lose carbon dioxide and metal fluoride and yield PFVEs [1]	
Major Commercial I	Products	-		
Name	FC-75			
CAS Number	335-36-4			
Composition	Mostly perfluorobutyltetral	nydrofurans [1]		
Use	Solvent [1]			
Name	Hexafluoropropylene oxide	e (HFPO)		
CAS Number	428-59-1			
Composition	C ₃ F ₆ O			
Production/Import volumes	Registered in Europe under tonnes per year. [2] 500 - <10,000t in the US	REACH with a production	n/import volume of 100–1000	

³¹ For more examples of compounds in this group and their associated information, one may search for the following IDs at the US EPA CompTox Chemicals Dashboard website: <u>https://comptox.epa.gov/dashboard</u>, namely DTXSID90893882.

Use	Starting material for the synthesis of hexafluoroacetone, perfluoropolyethers, and fluorinated vinyl ethers. [1]				
Uses					
Major applications	Perfluoroalkylether chemicals mentioned here and mixtures thereof (perfluorinated fluids) are used in the electronics industry, as immersion coolants for supercomputers and testing applications. [3]				
Knowledge gaps					
 Little information is available on perfluoroalkylethers that do not feature acids groups or are considered polymers. There is limited to no information on their degradation or reported occurrences in the environment. 					
References					

- [1] G. Siegemund et al., "Fluorine Compounds, Organic," Ullmann's Encycl. Ind. Chem., pp. 1–56, 2016.
- [2] European Chemicals Agency (ECHA), "Trifluoro(trifluoromethyl)oxirane Registration Dossier" [Online]. Available: <u>https://echa.europa.eu/registration-dossier/-/registered-dossier/5721</u>. [Accessed: 05-Dec-2019].
- [3] M. G. Costello, R. M. Flynn, and J. G. Owens, "Fluoroethers and Fluoroamines," in *Kirk-Othmer Encyclopedia of Chemical Technology*, vol. 11, Hoboken, NJ, USA: John Wiley & Sons, Inc., 2004, pp. 1–12.
- [4] U.S. EPA, Chemical Data Reporting (CDR), 2016. Available at <u>https://www.epa.gov/chemical-data-reporting/access-cdr-data</u>.

10. Perfluoroalkenes (a) and derivatives (b)

Chemical Information & Properties							
Identification and Terminology							
Name	Perfluoroalkenes	Perfluoroalkene derivatives ³²					
Other Names	Fluorinated Olefins; fluoroolefins						
Chemical Formula	$C_n F_{2n} (n > 2)^{33}$						
General Structure (linear isomers) (Examples of derivatives shown on the right taken from [1])	$F \xrightarrow{F}_{n} C \xrightarrow{F}_{n$	$\begin{array}{c ccccc} F & O & F & F & F \\ \hline F & F & F & F & F \\ CF_3 CF_3 F & CF_3 CF_3 F \\ CAS 88022-48-4 & CAS 120695-78-5 \end{array}$					
		$\begin{array}{c} CF_3, F_2, CF_3\\ & CF_3 \\ & CF_3 \\ & CF_3 \\ & CF_3 \\ & CAS \\ & 70829\text{-}87\text{-}7 \\ & (OBS, also see below under Major Commercial Products) \end{array}$					
US EPA CompTox Markush & Substance IDs	DTXSID201024683	DTXSID40897491, DTXSID20694127, DTXSID601020833					
Degradability, Mobility, Bioconcentration							
Degradation in the atmosphere	Atmospheric lifetimes: 6 d for C_3F_6 [1] Reaction rate constants with OH-radicals: 2.6 (C_3F_6) × 10 ⁻¹² cm ³ molecules ⁻¹ s ⁻¹ , yielding CF ₃ CFO and CF ₂ O, then enter the aqueous phase in 5–10 days, where they are eventually degraded to HF and TFA, and HF and CO ₂ , respectively. [2]						
Ozonolysis	Reaction with ozone under atmospheric conditions is slow [1], but perfluoroalkenes can be broken down via reductive ozonolysis [3].						
Biodegradation	OBS is non-readily biodegradable [4]						
Other degradation methods	OBS can be decomposed by photolysis combined with hydrogen peroxide [4]						
Synthesis							
Main Synthesis Method	Dehalogenation of halofluoroalkanes with zinc and an alcohol or dehydrohalogenation of haloalkanes with alcoholic alkali or by heating. Alternatively, addition of hydrogen halides to alkynes, decarboxylation of fluorocarboxylic acid salts, or pyrolysis of						

³² For more examples of compounds in this group and their associated information, one may search for the following IDs at the US EPA CompTox Chemicals Dashboard website: <u>https://comptox.epa.gov/dashboard</u>, namely DTXSID101010249, DTXSID401010250.

 $^{^{33}}$ According to the revised PFAS definition in the latest OECD PFAS Terminology report (https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/), tetrafluoroethylene (TFE; CF₂=CF₂) and hexafluorobutadiene (F₂C–CF=CF–CF₂) are not PFASs due to a lack of saturated fluorinated atoms.

		fluorohydrocarbons are also common synthesis methods. [5]						
Other sources		Perfluoroalkenes (such as C_3F_6 or C_4F_8) can also be released when fluoropolymers are incinerated and the polymers are degraded to release the monomers. [6]						
Industrial Prac	ctices	& Commerci	al Uses					
Major Commer	cial l	Products						
Name		Hexafluoropr	opene (HFP)					
CAS Number		116-15-4						
Use		Most importation the epoxide here.	tly in the production of copolymers, e.g. with TFE or VDF, also to produce xafluoropropylene oxide. [5]					
Production/Import volumesRegistered in tonnes per ye 5000 - <25,0		Europe under REACH with a production/import volume of 1000–10 000 ar. [7] 000t in the US in 2015 [8]						
Name		Sodium p-per	o-perfluorous nonenoxybenzene sulfonate (OBS)					
Composition	<i>ı</i> C ₉ F ₁₇ OC ₆ H ₄ S		O ₃ Na					
CAS Number	<i>ıber</i> 70829-87-7		-87-7					
Use		Additive for f [4]	ire-fighting foa	ighting foams; surfactant for oil production, mainly used in China [9],				
Production/Import 3500 tonnes/ volumes		3500 tonnes/y	/yr in China (reported in 2017) [9], [4]					
Degradation		Can be decom	nposed by UV/I	H_2O_2 or UV, w	hile in aqueous solution [4]			
Examples of re	port	ed occurrence	S					
Type of	(En	viron-	Detected in	Examples				
locations/ me samples		ntal) media	one or multiple regions	Location, year	Levels [minmax. (detection frequency)]	Ref.		
Non-detects are pg = picograms,	repor ng =	rted as below th nanograms, w	e value of the li w = wet weight	imit of detectio t, ND = not det	n (" <lod"). ected, NR = not reported</lod"). 			
Close to point sources		air surface water soil sediment	☐ one ⊠ multiple	China 2015 (close to new oilfield)	OBS: 9.9–110 ng/L (9/9)	[10]		
				China 2015 (close to old oilfield)	OBS: 10–3200 ng/L (26/26)			
Not close to specific point sources		air surface water soil sediment	⊠ one □ multiple	China 2015	OBS: <0.96–19 ng/L (NR/8)			
Knowledge gap	s		•	•		<u>.</u>		

- Little information is available on long-chain perfluoroalkenes and derivatives.

- Environmental monitoring data are missing.

References

- [1] OECD, "New Comprehensive Global Database of PFASs," [Online]. Available: <u>https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/</u> [Accessed: 24-Jul-2020]
- [2] G. Acerboni *et al.*, "Atmospheric degradation and global warming potentials of three perfluoroalkenes," *Atmos. Environ.*, vol. 35, no. 24, pp. 4113–4123, 2001.
- [3] K. I. Odinokov, I. F. R. Akhmetova, R. G. Savchenko, / I Y Bazunova, J. A. Yatykhov, and A. Y. Zapevalov, "Ozonolysis of perfluoroalkenes and perfluorocycloalkenes," 1997.
- [4] Y. Bao, Y. Qu, J. Huang, G. Cagnetta, G. Yu, and R. Weber, "First assessment on degradability of sodium p-perfluorous nonenoxybenzene sulfonate (OBS), a high volume alternative to perfluorooctane sulfonate in fire-fighting foams and oil production agents in China," *RSC Adv.*, vol. 7, no. 74, pp. 46948–46957, 2017.
- [5] G. Siegemund et al., "Fluorine Compounds, Organic," Ullmann's Encycl. Ind. Chem., pp. 1–56, 2016.
- [6] Z. Wang, I. T. Cousins, M. Scheringer, R. C. Buck, and K. Hungerbühler, "Global emission inventories for C₄–C₁₄ perfluoroalkyl carboxylic acid (PFCA) homologues from 1951 to 2030, part II: The remaining pieces of the puzzle," *Environ. Int.*, vol. 69, pp. 166–176, Aug. 2014.
- [7] European Chemicals Agency (ECHA), "Hexafluoropropene Registration Dossier" [Online]. Available: https://echa.europa.eu/registration-dossier/-/registered-dossier/15192. [Accessed: 13-Dec-2019].
- [8] U.S. EPA, Chemical Data Reporting (CDR), 2016. Available at <u>https://www.epa.gov/chemical-data-reporting/access-cdr-data</u>.
- [9] C. Wang *et al.*, "Bioaccumulation in the gut and liver causes gut barrier dysfunction and hepatic metabolism disorder in mice after exposure to low doses of OBS," *Environ. Int.*, vol. 129, pp. 279–290, Aug. 2019.
- [10] L. Xu *et al.*, "Discovery of a Novel Polyfluoroalkyl Benzenesulfonic Acid around Oilfields in Northern China," *Environ. Sci. Technol.*, vol. 51, no. 24, pp. 14173–14181, 2017.
| Chemical Information & Inherent Properties | | | | | | |
|--|--|--|--|--|--|--|
| Identification and Te | erminology ³⁵ | | | | | |
| Name | Hydrofluorocarbons | Hydrofluoroethers | Hydrofluoroolefins | | | |
| Other Names | | | Fluorinated olefins [1] | | | |
| Acronym | HFCs | HFEs | HFOs | | | |
| Chemical Formula
(those with at least
one saturated fully
fluorinated carbon
atom) | $C_nH_xF_y$ with $x + y = 2n + 2$ | $C_nH_xF_yOC_mH_pF_q$ with $x + y = 2n + 1$;
p + q = 2m + 1;
x + y + p + q = 2(n + m + 1) | $C_n H_x F_y$
with $x + y = 2n$ | | | |
| Degradability, Mobi | lity, Bioconcentration | | | | | |
| Atmospheric lifetime | 13.4 years (HFC-134a;
CH ₂ FCF ₃) [2] | Between 0.8 (HFE-7200;
C ₄ F ₉ OCH ₃) and 165 (HFE-
125; CHF ₂ OCF ₃) years [3] | ca.10 d (HFO-1234yf;
CF ₃ CF=CH ₂) [4,5] | | | |
| | Atmospheric reactions with OH radicals can yield PFCAs. [1], [6] For HFCs and HFOs used as refrigerants and foam blowing agents, some yield TFA (trifluoroacetic acid) and not longer-chain PFCAs. [7] [8] [9] | | | | | |
| Ozone Depletion
Potential (ODP) | Between 10 ⁻⁵ and 10 ⁻³
(varying between studies)
[10]. Atmospheric changes
in temperature and
circulation arising from
HFC emissions lead to a
weak, indirect depletion of
stratospheric ozone [11]. | Negligible [12] | Negligible [9] | | | |
| 100 Year Global
Warming Potential
(GWP) | Between 1300 (HFC-134a)
and 8060 (HFC-236fa;
CF ₃ CH ₂ CF ₃) [2] | Between 60 (HFE-7200)
and 14 000 (HFE-125) [3] | <1 (HFO-1234yf) [2]
2 (HFO-1336mzz;
CF ₃ CH=CHCF ₃) [2] | | | |
| Biodegradation | (The commercially relevant) | HFCs, HFEs, and HFOs are g | ases with low water | | | |
| Bioconcentration | solubility. They almost entirely partition into the atmosphere, with atmospheric degradation as a major degradation process. For this reason and others, there are limited data on biodegradation or bioconcentration. | | | | | |
| Synthesis | | | | | | |
| Main Synthesis | Addition of hydrogen | Synthesized from alkoxides | Dehalogenation of | | | |

11. Specific hydrofluoro-carbons (a), -ethers (b), and -olefins (c) ³⁴

³⁴ Note that not all HFCs, HFEs and HFOs are included here, but only those that contain at least one perfluorinated methyl (–CF₃) or methylene (–CF₂–) group. Many HFCs and HFOs used as refrigerants and foam blowing agents do not fall under PFAS according to the revised PFAS definition in the latest OECD PFAS Terminology report (https://oe.cd/2M9), e.g. those having CF₂XY (where X and Y \neq F) structures.

³⁵ Common naming conventions have been established for HFCs, HFEs, HFOs and many other fluorinated gases; for more details, see for example <u>https://www.fluorocarbons.org/wp-content/uploads/2020/06/EFCC-NamingNumbering A4 V01-23062020.pdf; https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32014R0517&from=EN.</u>

Method	fluoride to olefins or alkynes; exchange of chlorine for fluorine, via hydrogen fluoride or metal fluorides; addition of hydrogen to perfluoroalkenes; decarboxylation of perfluorocarboxylates; electrochemical fluorination. [1]	or phenoxides and fluoroolefins. [1]	haloalkanes; dehydrohalogenation of hydrogen-containing haloalkanes; addition of hydrogen halides to alkynes; decarboxylation of fluorocarboxylic acids; pyrolysis of fluorohydrocarbons. [1]
Possible Impurities			CHCl ₂ F and hexafluoropropene in the production of tetrafluoroethylene. [1]
Industrial Practices	& Commercial Uses		
Major Commercial I	Products		
Name(s)	1,1,1,2-Tetrafluoroethane		
Trade Name(s)	HFC-134a / R-134a / Freon 1 134a / Norflurane	134a / Forane 134a / Genetron	134a / Florasol 134a / Suva
Chemical Formula	CH ₂ FCF ₃		
CAS Number	811-97-2		
Use	See Major applications below	w.	
Production/Import volumes	Between 1990 and 1995, 159 the EU under REACH with a year [13]. 50,000 - <125.000t in the U	9 500 t have been produced [1] a production/import volume of JS in 2015 [14]	. HFC-134a is registered in 10 000 – 100 000 tonnes per
Name(s)	2,3,3,3-Tetrafluoropropene		
Trade Name(s)	HFO-1234yf / R-1234yf / Oj	pteon YF / Solstice YF / HFC-	1234yf
Chemical Formula	CH ₂ =CFCF ₃		
CAS Number	754-12-1		
Use	See Major applications below	W.	
Production/Import volumes	Registered in the EU under F 10 000 tonnes per year. [15] 500 - <10,000t in the US in	REACH with a production/imp 2015 [14]	ort volume of 1000 –
Uses			
Major applications	HFCs are mostly used as substitutes for CFCs and HCFCs: in refrigeration and air-conditioning, as propellants in aerosols, and as foaming agents in closed cell foams (e.g. for building insulation), as	HFEs replace HFCs in some of the applications mentioned, due to their lower global warming potential [6]. Some HFEs are also used as inhalation anesthetics. [1]	Replacements for HFCs and HFEs [17]. Production of fluorinated polymers and inert fluids [1].

ENV/CBC/MONO(2022)1 | 75

		well as in fire extinguishing other applicat [7]. HFC-1344 227ea (CF ₃ CF been used as p for metered de	systems, and ions [1], [16], a and HFC- FHCF ₃) have propellants ose inhalers				
		[7]					
Regulatory Sta	atus						
US		Under the SNAP (Significant New Alternatives Policy) Program the US EPA identifies and approves climate-friendly alternatives for ozone-depleting substances. Federal Agencies have to report their greenhouse gas emissions, including HFC emissions, and have to procure alternatives to HFCs with high global warming potentials, if possible. [16]. Several US states have implemented stricter regulations to reduce HFC emissions. [18]. In December 2020, the US passed the American Innovation and Manufacturing Act, mandating an 85 % phasedown of HFCs by 2036, consistent with the Kigali Amendment and other emission-reducing measures [19]					
European Unio	n	The F-gas Regulation 517/2014 limits the total amount of fluorinated greenhouse gases (including HFCs, perfluorocarbons, Sulphur hexafluoride and other greenhouse gases that contain fluorine, listed in Annex I; note that HFEs and HFOs are not addressed by this regulation) that can be sold in the EU, with the goal to cut emissions by two-thirds by 2030 compared to 2014. Use of these gases is banned where less harmful alternatives are available, and emissions are to be prevented by proper servicing of equipment and recovery of the gases at the end of the product life cycle. The regulation also sets requirements of reporting on production, import, export, feedstock use and destruction of the substances listed in Annexes I or II (including HFO, HFEs and other perfluorinated compounds). [20] The use of refrigerants in new cars (in heating, ventilation and air conditioning), which have global warming potentials higher than 150 (which includes HFC-134a) is prohibited					
Canada		HFCs are re Alternatives I obligations un rules concerni	gulated pursua Regulations. The oder the Montre ng HFCs and co	ant to the Oz ne purpose of t cal Protocol, ind ertain products	cone-depleting these Regulation cluding the Kiga containing or de	Substances and Halo ns is to implement Ca ali amendment, by sett esigned to contain HFG	ocarbon anada's ting out Cs [21].
International e	efforts						
The Kigali Amendment to the Montreal Protocol specifically addresses HFCs (not HFEs and HFOs), with the goal to reduce HFC production and consumption by 85 % by 2036 for developed countries, by 80 % by 2045 for most developing countries and by 85 % by 2047 for a small group of developing countries (reduction based on baseline levels). [22] The Amendment came into effect in 2019, with some countries that are parties to the Protocol yet to ratify the amendment. [18] The Scientific Assessment Panel and the Environmental Effects Assessment Panel to the Montreal Protocol provide regular updates on emissions and environmental fate of HFCs [23, 24].							
Examples of r	eport	ed occurrence	S				
Type of	(Env	ironmental)	Detected in	Examples			
locations/ samples	medi	a	one or multiple regions	Location, year	Levels [min frequency)]	-max. (detection	Ref.
Non-detects are reported as below the value of the limit of detection (" <lod").< td=""></lod").<>							

$ppt = parts \ per \ trillion, \ ppt_v = parts \ per \ trillion \ (volume \ fraction), \ ND = not \ detected, \ NR = not \ reported$							
Not close to specific point	air surface water	☐ one ⊠ multiple	China 2010	HFC-134a: 87 ppt _v (<i>mean</i>) (NR/92)	[25]		
sources	soil sediment		US 2010	HFC-134a: 65.4 ppt _v (<i>mean</i>) (NR)			
			Global surface	HFC-125: 20.1–20.8 ppt (means derived by different methods)	[23]		
			mean 2016	HFC-134a: 89.3–92.1 ppt (means derived by different methods)			
				HFC-143a (CH ₃ CF ₃): 19.0–19.3 ppt (<i>means derived by different</i> <i>methods</i>)			
				HFC-245fa (CHF ₂ CH ₂ CF ₃): 2.43 ppt (<i>mean</i>)			
				HFC-365mfc (CF ₃ CH ₂ CF ₂ CH ₃): 0.87–1.0 ppt (<i>means derived by</i> <i>different methods</i>)			
				HFC-227ea: 1.17–1.24 ppt (means derived by different methods)			
				HFC-43-10mee (CF ₃ CHFCHFCF ₂ CF ₃): 0.27 ppt (<i>mean</i>)			
				HFC-236fa: 0.15 ppt (mean)			
Urban area	ir ☐ air ☐ surface water	⊠ one □ multiple	Switzerland 2016	HFO-1234yf: <0.003–approx. 9.2 ppt (NR)	[23]		
	soil sediment			HFO-1234ze (<i>trans</i> - CHF=CHCF ₃): <0.003–approx. 25 ppt (NR)			
Remote regions	ir ☐ surface water	☐ one ⊠ multiple	Swiss alps 2004	HFC-134a: approx. 30–approx. 130 ppt (NR)	[26]		
	soil sediment		Italian alps 2004	HFC-134a: approx. 30–approx. 140 ppt (NR)			
			Swiss alps 2016	HFO-1234yf: <0.003–approx. 8.2 ppt (NR)	[23]		
				HFO-1234ze: <0.003–approx. 10 ppt (NR)			
Knowledge ga	ps						
- Environmental concentrations of less commonly known HFEs and some of the newer HFOs.							
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 $ppt = parts per trillion ppt_{v} = parts per trillion (volume fraction) ND = not detected NR = not re$

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12. Side-chain fluorinated aromatics

Chemical Information & Inherent Properties				
Identification and Te	erminology			
Name	Side-chain fluorinated aromatics			
Other Names	Aromatic compounds with perfluorocarbon moieties on the side chain(s)			
Chemical Formula	e.g. $C_6R_5C_nF_{2n+1}$			
Exemplary Structure (linear isomers)	$R^{2} \xrightarrow{R^{1}} F$ $R^{3} \xrightarrow{R^{4}} R^{5}$ Note that fluorinated side chains may also be attached via other types of bonds, e.g. via an ester bond.			
General remarks	Benzotrifluorides (e.g. $C_6R_5CF_3$, n=1) are a group of commercially relevant side-chain fluorinated aromatics [1]. As there is little information on other side-chain fluorinated aromatics, this fact card focuses on benzotrifluorides and their derivatives.			
Degradability, Mobi	lity, Bioconcentration			
Biodegradation	No biodegradation of benzotrifluoride (BTF) in activated sludge after 28 days [2]; Complete mineralization of fluorinated drugs is rare. Fluoxetine (see in section on commercial products below) is not eliminated by conventional wastewater treatment, but is removed via ozone or active carbon [3]–[5]. Fluometuron (see in section on commercial products below) is not readily biodegradable [6].			
Bioaccumulation	BCF (aquatic species) of BTF = 58 [2] BCF (fish) of fluoxetine = 8.8–260 (estimated) [7] BCF (fish) of norfluoxetine = 80–650 (estimated) [7] BCF (mussels) of fluoxetine = 125–1347 [8]			
Synthesis				
Main Synthesis Method	Halogen exchange using hydrogen fluoride [1]: $C_6H_5CCl_3 + 3 HF \longrightarrow C_6H_5CF_3 + 3 HCl$			
Possible Impurities	Typically, a yield between 70–90% is obtained, depending on the specific process conditions. It remains unclear what side products and possible impurities are generated. [1]			
Industrial Practices	& Commercial Uses			
Major Commercial I	Products			
Name	Benzotrifluoride / α , α , α -trifluorotoluene / trifluoromethylbenzene			
Acronym	BTF			

Chemical Form	nula	C ₆ H ₅ CF ₃						
CAS Number		98-08-8						
Use		Intermediate i	in the synthesis	of dyes, pestic	ides, and pharmaceuticals.			
Production/Imp volumes	oort	Registered in year. [2]	the EU under R	EACH with a p	production/import volume of 0–10 tor	ines per		
Name		4-chlorobenzo	otrifluoride / Pa	rachlorobenzot	rifluoride			
Acronym		4CBTF / PCE	BTF					
Trade Name(s)		Oxsol 100 [9]						
Chemical Form	nula	C ₆ H ₄ ClCF ₃						
CAS Number		98-56-6	98-56-6					
Use		Solvent, especially for paint and ink formulations; cosmetic stain remover; aerosc inhibitor [9]			sol rust			
Production/Imp volumes	oort	Registered in the EU under REACH with a production/import volume of $100-1000$ tonnes per year. [10] 5 000 - <25 000t in the US in 2015 [16]						
Name		Fluoxetine						
Trade Name(s)		(active ingredient in) Prozac [8]						
Chemical Form	ıula	C17H18F3NO						
CAS Number		54910-89-3						
Use		Antidepressar	nt, specifically s	selective seroto	nin reuptake inhibitor (SSRI) [8]			
Production/Imp volumes	oort	Volumes sold	in 2003 and 20	004: 3.7 t/yr (Fr	ance), 4.8 t/yr (UK), 4.2 t/yr (Spain)	[4]		
Name		N,N-dimethyl	-N'-[3-(trifluor	omethyl)-pheny	rl]-urea			
Trade Name(s)		Fluometuron						
Chemical Form	nula	$C_{10}H_{11}F_3N_2O$						
CAS Number		2164-17-2						
Use		Herbicide, esp	pecially used in	cotton product	ion [1], [11]			
Production/Imp volumes	oort	Registered in per year. [6]	the EU under F	REACH with a	production/import volume of 10–100) tonnes		
Uses								
Major applicationsBenzotrifluorides derivatives are used as dyes, where the trifluoromethyl group impro color clarity, as well as pharmaceuticals [12] and pesticides, since the trifluorome group accelerates absorption [1]. BTF and PCBTF are also used as organic solvents [aproves omethyl ats [13].				
Examples of r	eport	ed occurrence	S					
Type of	(Env	ironmental)	Detected in	Examples				
locations/ samples	medi	a	one or multiple regions	Location, year	Levels [min. –max. (detection frequency)]	Ref.		

ng = nanogram	is, ww = wet weight, I	VD = not aetect	ea, NR = not re	sportea	
Close to point sources	☐ air ☐ surface water ☐ soil ⊠ sediment	☐ one ⊠ multiple	US (close to WWTP effluent) 2010 (year of publication)	Fluoxetine: 17.4 ng/g ww (mean) (NR/12)	[8]
	Groundwater	1	Italy 2008 (Valleagno	BTF: 98 ng/L (mean) (3/3)	[15]
			area, site of chemical	4-Chloro-BTF: 11900 ng/L (mean) (3/3)	
			spill in 1977)	3,4-dicholoro-BTF: 6400 ng/L (mean) (3/3)	
				2,4-dicholoro-BTF: 220 ng/L (mean) (3/3)	
				3-nitro-BTF: 430 ng/L (<i>mean</i>) (3/3)	
				3-amino-BTF: 580 ng/L (mean) (3/3)	
				3-amino-4-chloro-BTF: 2600 ng/L (mean) (3/3)	
				3-nitro-4-chloro-BTF: 5900 ng/L (mean) (3/3)	1
Not close to specific point sources	□ air ☑ surface water □ soil □ sediment	☐ one ⊠ multiple	Portugal 2013–2014	Fluoxetine: 2.01–19.5 ng/L (55/55)	[14]
WWTP	☐ effluent ⊠ influent ☐ sludge	☐ one ⊠ multiple	Portugal 2013–2014	Fluoxetine: 5.21–17.8 ng/L (55/55)	[14]
	effluent	1	Portugal 2013–2014	Fluoxetine: 10.5–34.0 ng/L (55/55)	[14]
	sludge		US 2010 (year of publication)	Fluoxetine: 118.8 ng/L (mean) (NR/6)	[8]
Wildlife	Freshwater mussels (<i>Elliptio</i> <i>complanata</i>) at WWTP effluent	☐ one ⊠ multiple	US 2010 (year of publication)	Fluoxetine: 79.1 ng/g ww (mean) (NR)	[8]
Knowledge ga	ps				

- Current production volumes are unknown, especially outside the EU.

- Environmental monitoring data are sparse.

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13. Fluoropolymers

Key publications: Dams, Rudy, and Klaus Hintzer. 2017. "Chapter 1. Industrial Aspects of Fluorinated Oligomers and Polymers." In *Fluorinated Polymers: Volume 2: Applications*, edited by Bruno Ameduri and Hideo Sawada, 1–31. Royal Society of Chemistry. <u>https://doi.org/10.1039/9781782629368-00001</u>.

Ebnesajjad, S., Introduction to Fluoropolymers – Materials, Technology and Applications. Plastics Design Library (PDL) Handbook Series. Elsevier. 2011

Chemical	Informat	ion & Inhe	rent Prope	erties				
Identificat	ion and T	erminology						
Name		Fluoropolyn	ners					
Other Nam	es	Fluoroplasti	cs					
Chemical I (Examples)	Formula	$(C_2F_2)_n$ (PTH)	FE) / (C ₂ H ₂]	F ₂) _n (PVDF	F, ETFE)			
General St. (Examples, PTFE, righ	ructure left: ht: FEP)	²) $F = \begin{pmatrix} F \\ C \\ F \\$						nes (as shown
Examples o	of major fli	voropolymer	s (adapted j	from [1])			_	
		TFE Co-	polymers =CF ₂			Homopolymers		
+	+	+	+	+	+			
PPVE	HFP	Ethene	HFP	CTFE	FC=CF	TFE	CTFE	VDF
F ₂ C=CF O C ₃ F ₇	F ₂ C=CF CF ₃	H ₂ C=CH ₂	F ₂ C=CF CF ₃ +	F ₂ C=CFCI +	R _f	F ₂ C=CF ₂	F ₂ C=CFCI	F ₂ C=CH ₂
			VDF	Ethene				
	I		F ₂ C=CH ₂	H ₂ C=CH ₂		1		
↓ PFA	↓ FEP	↓ ETFE	↓ THVs	↓ ECTFE	↓ Teflon AF	↓ PTFE	↓ PCTFE	↓ PVDF
Acronyms: 7	TFE = tetra	fluoroethylene;	PPVE = per	fluoropropylvi	nylether; HFP	= xexafluoroprop	pylene; VDF = v	/inylidene fluoride;
CTFE = chlore	lity Mobi	ie; VF = vinyl flu	ioride					
Degradabi					• • • .	1 4	1	
Abiofic deg	radation	Fluoropolyn	iers exhibit	high chem	ical resistan	ce and weather	resistance. [2]	
Thermal de	<i>Thermal degradation</i> Fluoropolymers are stable up to high temperatures, e.g., PTFE is stable up to 250 °C. Thermal degradation begins slowly at higher temperatures and results mainly in monomer formation (e.g. tetrafluoroethylene), although the formation of hydrogen fluoride is also possible at higher temperatures [2]–[4]. Also, the formation of C_2 – C_{14} per- and polyfluoroalkyl carboxylic acids have been reported. [5], [6]							
Synthesis								

Main Synthesis Method	Free-radical polymerization, either in aqueous suspension or aqueous emulsion. The latter often requires fluorinated emulsifiers (fluorosurfactants) as polymerization aids. Water soluble peroxides or trialylboron catalysts are used to initiate the polymerization process. [7], [8] In some cases, free-radical solvent polymerization can also be utilized. ³⁶					
Possible Impurities	Residues of fluorosurfactants, used as processing aids in the emulsion polymerization process, can potentially remain in the final products and can be released during later life-cycle stages [8]. Low molecular weight oligomers are also produced and can be released to the environment [9].					
Industrial Practice	s & Commercial Uses					
Major Commercial	l Products					
Name(s)	Polytetrafluoroethylene (PTFE)					
Trade Name(s)	Teflon					
Chemical Formula	-[CF ₂ -CF ₂] _n -					
CAS Number	9002-84-0					
Use	Chemical processing, resistant components & coatings, pipes, fittings, linings, tapes, seals, filters, wire & cable insulation, laminates, waterproof & stain repellent clothing, architectural coatings, printing, cookware, fabrics, biomedical devices [8]					
Production/Import volumes	Global production in 2013: 200 000 tonnes; 15 000 tonnes produced in Europe [10] Global demand in 2016: 160 000 tonnes [3]					
Name(s)	Polyvinylidene fluoride (PVDF)					
Chemical Formula	-[CH ₂ -CF ₂] _n -					
CAS Number	24937-79-9					
Use	Fluid handling systems, valves, pumps, water piping, resistant paints, architectural coatings, wire & cable insulation, electronic components, solar panels, printing [7]					
Production/Import volumes	Global consumption in 2012: 35 500 tonnes [11] Global demand in 2016: 33 000 tonnes [3]					
Name(s)	Fluorinated ethylene propylene (FEP)					
Chemical Formula	$-[CF_2-CF_2]_n-[CF_2-CF(CF_3)]_m-$					
CAS Number	25067-11-2					
Use	Chemically resistant components & coatings, plenum cable insulation [7]					
Production/Import volumes	Global demand in 2016: 40 000 tonnes [3]					
Name(s)	Perfluoroalkoxy alkane (PFA) / Perfluoroalkoxy polymer					
Chemical Formula	$-[CF_2-CF_2]_n-[CF_2-CF(OR_F)]_m- (R_F = fluorinated group)$					
CAS Number	26655-00-5 / 31784-04-0					
Use	Chemical processing, resistant components and fittings, electrical insulation, industrial & architectural coatings, semiconductor manufacturing [4], [7]					

³⁶ According to information provided by representatives of the manufacturing industry.

Uses								
Major	<i>Major applications</i> Chemically resistant coatings and linings in chemical processing (e.g. pipe linings, tank reaction vessels, valves, membranes), electrical insulation, nonstick coatings (e.g. for cookware), high-performance textiles, medical devices (such as catheters, heart patche sutures, and others) [3]							
Regula	ntory Statu	S						
Generc	<i>Teneral remarks</i> In the US, fluoropolymers and their safety are reviewed in the context of specific applications (e.g. as food contact materials or for use in a medical context) by the US EPA, the US FDA, and the US Consumer Product Safety Commission, and similarly in the EU [2], [3].							
Examp	oles of repo	orted occurrences						
Туре о	of	(Environmental)	Detected in	Examples				
locatio sample	ns/ es	media	one or multiple regions	Location, year	Levels [min. –max. (detection frequency)]	Ref.		
Non-de pg = p	etects are re icograms, r	eported as below the $ng = nanograms$, wy	e value of the lir v = wet weight,	nit of detection ND = not detection	(" <lod"). cted, NR = not reported</lod"). 			
Remote	e regions	☐ air ☐ surface water ☐ soil ⊠ sediment	⊠ one □ multiple	Arctic ocean 2015	0.89–9.43 particles/kg sediment (9/9; PTFE)	[12]		
Knowl	edge gaps							
- Quan	tified envi	conmental occurren	ces of fluoropo	lymers, especi	ally others than PTFE, are largely	unknown.		
- Produ	uction volu	mes are not public	ly available.					
- Limi molecu	ted inform 11ar weight	ation is available range, molar ratio	regarding chen and compositio	nical identities	s of commercial PFPE products units, impurity content, function	(including al groups).		
- More from f major	informatic luoropolyn historical s	on is needed on how ners throughout the ource of PFOA in	v much PFCAs eir life cycle, a the environmer	and other orga lthough fluoro nt.	nofluorine compounds are current polymer manufacturing was show	ly emitted wn to be a		
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14. Fluoroelastomers³⁷

Key publications: Worm, A. T.; Gorrtaert, W., Fluorocarbon Elastomers. *Encyclopedia of Polymer Science & Engineering* 2015. <u>https://doi.org/10.1002/0471440264.pst137</u>

Améduri, B.; Boutevin, B.; Kostov, G., Fluoroelastomers: Synthesis, properties and applications. Progress in Polymer Science (Oxford) 2001, 26, (1), 105-187. https://www.sciencedirect.com/science/article/pii/S0079670000000447?via%3Dihub.

Chemical Information & Inherent Properties							
Identification and Terminology							
Name	Fluorocarb	on elastome	rs	Fluorosilicones	Fluorinated polyphosphazenes		
Other Names				Fluorocarbon- modified silicones			
Acronym	FKM			FLS	PNF elastomers		
General structures (exemplary) Schematic overview (adapted from [21])	Copolymers of VDF $(C_2H_2F_2)$ & HFP (C_3F_6) Terpolymers of VDF, HFP & TFE (C_2F_4) Terpolymers of VDF, TFE & PMVE (C_3F_{60}) [19]			$ \begin{array}{c} $	$ \begin{array}{c} $		
	TFE $F_2C=CF_2$ + VDF $F_2C=CH_2$ + HFP $F_2C=CF_CF_3$ + Cure package \downarrow FKM	+ Propene H ₂ C=CH CH ₃ + Cure package ↓ FEPM	+ PMVE $F_2C = CF$ O CF_3 + fct. comonomer + Cure package \downarrow FFKM				
Acronyms: TFE = Tetrafluo FEPM = Tetrafluoroethylene	roethylene; VDF propylene; PM	F = Vinylidene f VE = Perfluoron	luoride; HFP = Hexa nethylvinylether; FFI	fluoropropylene; FKM = fluoroc KM = perfluoro-elastomers	arbon elastomers;		

³⁷ Fluoroelastomers are also fluoropolymers, but have rather different physical and chemical properties from those presented in the previous fact card on fluoropolymers. Therefore, they are made into a separate fact card here.

Degradability, Mobil	lity, Bioconcentration		
Stability	Mostly resistant towards light, ozone, heat, solvents, aggressive chemicals, and combinations thereof. Heat resistant until 250 °C. In general, stability increases with fluorine content. [3] FKM is more susceptible to alkaline degradation, e.g. FKM was found to degrade slowly (>12 weeks) in a warm alkaline environment (10% NaOH, 80 °C). [4], [5] Some "base-resistant" FKMs and FEPM resist degradation in high pH environments. ³⁸	Inert under normal conditions, but decompose at extreme pH-values or at high temperatures, in which case toxic fluorinated compounds such as 3,3,3-trifluoropropion- aldehyde are produced. [6]	Depolymerization occurs at temperatures above 300 °C. Fluorinated polyphosphazenes are very resistant to combustion. [7]
Synthesis			
Main Synthesis Method	High-pressure, free-radical aqueous emulsion polymerization, with organic or inorganic peroxy- compounds as initiators. Fluorosurfactants (or non-fluorinated surfactants) can be added as emulsifiers, and ethyl acetate, methanol, acetone, or others can be used as chain-transfer agents. For curing, bisphenol cross-linking agents are added as well as a cure accelerator, such as triphenylbenzylphosphonium chloride. [1], [8]	Base-catalyzed ring- opening polymerization of cyclic trimers, obtained through hydrolysis of the corresponding dichlorosilane. [1]	First, ring-opening polymerization of the cyclic trimer (NPCl ₂) ₃ or living cationic condensation polymerization of a phosphoranimine yields poly(dichloro- phosphazene). In a second step, chlorine is replaced with fluoro-organic side groups. [7]
Possible Impurities	Residues of processing aids can potentially remain in the final product.		
Industrial Practices	& Commercial Uses		
Major Commercial I	Products		
Production/Import volumes	Total fluoroelastomers consumption gl 40% of which in the US, 30% in Europ Japan). [8]	obally: approximately 10 be, 20% in Japan, and 10%	000 t/yr as of 2001, 5 in Asia-Pacific (excl.
Name(s)	1,1-difluoroethylen-hexafluoropropene polyvinylidenefluoride/hexafluoroprop Vinylidene fluoride-hexafluoropropyle	polymer / ene [9], [10] ne copolymer [16]	
CAS Number	9011-17-0		
Trade Name(s)	DAI-EL; Dyneon; Tecnoflon, Viton		
Use	O-ring and oil seal applications in high	-heat environments [17]	

³⁸ According to information provided by representatives of the manufacturing industry.

Name(s)	Vinylidene fluoride-hexafluoropropyle Poly(TFE-ter-VDF-ter-PMVE)	ne-tetrafluoroethylene ter	polymer		
CAS Number	25190-89-0	25190-89-0			
Trade Name(s)	Viton GLT [12] DAI-EL; Dyneon; Teo	enoflon; Viton			
Use	Transfer or compression molded autom [13]. Extruding fuel tubing and hose [2]	notive fuel, chemical, and p 20].	petroleum industry seals		
Name(s)	Vinylidene fluoride-tetrafluoroethylene Poly(TFE-ter-PMVE-ter-VDF)	e-perfluorovinyl methyl et	ther terpolymer		
CAS Number	56357-87-0				
Trade Name(s)	DAI-EL LT [17], Tecnoflon-PL [12];	Viton GLT [12]			
Use	O-rings, seals, gaskets used in the auto	motive, aerospace, and en	ergy industries. [14]		
Name(s)	Fully fluorinated copolymers of tetrafle Poly(TFE-ter-PMVE-ter-8CNVE)	uoroethylene and a perflue	oroalkyl vinyl ether		
Trade Name(s)	DAI-EL Perfluor [17]; Kalrez [12]; Te	cnoflon PFR, PFR-HT, Pl	FR-LT		
Composition	Perfluorinated rubbers of polymethylene type having all fluoro, perfluoroalkyl or perfluoroalkoxy substituent groups on the polymer chain (e.g. TFE and PMVE).				
Use	O-rings, seals, gaskets used in the automotive, aerospace, and energy industries. [14] O-rings, seals, gaskets and tubing used in the semiconductor processing industry [17]				
Names(s)	Copolymers of tetrafluroethylene and propylene [18]				
Trade names(s)	Aflas				
Use	O-rings, seals, gaskets and wire covering for the oil and gas, chemical process, industrial equipment, food handling, pharmaceutical, heavy duty diesel and automotive industries. [18]				
Name(s)	1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1,1,2,2,3,3-heptafluoro-3-((1,2,2-trifluoroethenyl)oxy)propane and 1,1,2,2-tetrafluoroethene				
CAS Number	63654-41-1				
Use	Wire coating and small diameter transp	parent tubing. [12]			
Uses					
Major applications	cationsMainly in ground transportation, i.e. engine oil seals, fuel system components, and drive-train seals. Also in the aerospace industry, in industrial hydraulic and pneumatic applications as well as the chemical processing industry and semiconductor manufacturing. [8], [15]Fuel-resistant elastomers, anti- graffiti and antifouling coatings, silicone pressure-sensitive adhesive release liners. [6]Fibers and nanofibers, impar 				
Knowledge gaps					
- Specific production	volumes are not publicly available.				

- Environmental monitoring data are not available for these compounds.

- Limited information is available regarding chemical identities of commercial products (including molecular weight range, molar ratio and composition of monomer units, impurity content, functional groups) and their life cycle, including possible releases of low molecular weight compounds.

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15. Perfluoropolyethers

Key publications: Moffett, et al., Perfluoroalkylpolyethers. In *Synthetics, Mineral Oils, and Bio-Based Lubricants. Chemistry and Technology*, Rudnick, L. R., Ed. Taylor & Francis, 2020. <u>https://doi.org/10.1201/9781315158150</u>.

Chemical Informati	on & Inherent Properties
Identification and Te	erminology
Name	Perfluoropolyethers
Acronym	PFPEs
An example of general structure (linear isomer examples) [1]	$F \longrightarrow \begin{bmatrix} F & F \\ C & -C \\ F & F \end{bmatrix} = \begin{bmatrix} F & F \\ C & -C \\ F & F \end{bmatrix} = \begin{bmatrix} F & F \\ C & -C \\ F & F \end{bmatrix} = \begin{bmatrix} F & F \\ C & -C \\ F & F \end{bmatrix} = \begin{bmatrix} F & F \\ C & -C \\ C & -C$
	Note: monomer units distributed randomly along the polymer backbone. In different PFPEs, different monomer units may present.
Degradability, Mobil	lity, Bioconcentration
Stability	Thermally stable, non-flammable, chemically resistant, resistant to ionizing radiation, non-volatile (up to 350 °C) [2]
Synthesis	
Main Synthesis Method	Anionic ring opening polymerization or UV-catalysed radical oxopolymerization (e.g. copolymerization of tetrafluoroethylene with O ₂) [1], [2]
Industrial Practices	& Commercial Uses
Major Commercial I	Products
Name(s)	Poly[oxy[trifluoro(trifluoromethyl)-1,2-ethanediyl]], α -(1,1,2,2,2-pentafluoroethyl)- ω -[tetrafluoro(trifluoromethyl)ethoxy]-
Trade Name(s)	Krytox PFPE High Performance Lubricant (60–100% of total product), Krytox Sodium Nitrite Inhibited PFPE/PTFE Greases (71–80% of total product) [3]
Chemical Formula	$-[OCF(CF_3)CF_2OCF(CF_3)CF_2OCF(CF_3)CF_2]-$
CAS Number	60164-51-4
Use	Nonflammable, stable and inert lubricant for applications in the aerospace and nuclear industries. [4]
Name(s)	Diphosphoric acid, polymers with ethoxylated reduced methyl esters of reduced polymerized oxidized tetrafluoroethylene
Trade Name(s)	Possibly Fomblin HC/P2-1000 [3]
CAS Number	200013-65-6
Use	Lubricant, and water and oil repellent in paper products and food packaging. [3]
Production/Import volumes	Produced or imported in volumes of over 11 340 kg in the US. Estimated value of dutiable imports to the US by 2017: 13 000 000 \$ [3]

Name(s)	1-Propene, 1,1,2,3,3,3-hexafluoro-, oxidized, polymd.
Trade Name(s)	Fomblin Y (also in Fomblin HC, Fomblin Y LVAC, Galden HT-90 Assay, Solkatherm SES 36) [3]
Chemical Formula	$-[CF(CF_3)CF_2OCF_2CF(CF_3)CF_2OCF_2CF(CF_3)CF_2OCF_2]-$
CAS Number	69991-67-9
Use	As a lubricant, welding and soldering agent, and in personal care products (cosmetics) [3]
Production/Import volumes	0.5 tonnes used in Sweden in 20170.3 tonnes used in Denmark in 2016 [3]
Name(s)	Ethene, 1,1,2,2-tetrafluoro-, oxidized, polymd.
Trade Name(s)	Fomblin Z60, Fomblin Z-15, FOMBLINCR 862 (50 - 55% of total product) [3]
CAS Number	69991-61-3
Name(s)	Tetrafluoroethylene, oxidized, oligomers, reduced, methyl esters, reduced, reaction products with ethylene oxide
Trade Name(s)	Fluorolink E10-H
CAS Number	162492-15-1
Use	Non-stick coating [3]
Name(s)	Hexafluoropropene, oxidized, oligomers, reduced and hydrolyzed
Trade Name(s)	Carbaflo XTR S5 F80 (1–2,4% of total weight) [3]
CAS Number	161075-14-5
Use	Lubricant used in automotive industry, also corrosion inhibitor and used in surface treatment applications effective in sub-zero temperatures. [3]
Production/Import volumes	Estimated value of dutiable imports to the US by 2017: 2 000 000 \$ [3]
Trade Name(s)	Fluorolink AD1700
Chemical Formula	$XCF_2O-(CF_2CF_2O)_m(CF_2O)_n-CF_2X$ where $X = CH_2OCOCH=CH_2$
Use	Used as additive for coatings, in battery systems and smart devices [3]
Trade Name(s)	Optool DSX
Chemical Formula	$CF_3CF_2CF_2O$ - $(CF_2CF_2CF_2O)_n$ - CF_2CF_2X where $X = CH_2CH_2Si(OR)_3$
Use	Used in anti-smudge coatings [3]
Uses	
Major applications	Mainly high performance lubricants for engines and machinery [2], but also as surface treatments for natural stone, metal, glass, plastic, textiles, leather, and paper, as well as paperboard treatment for food-contact applications [1].
Knowledge gaps	
- Production and use	volumes are not publicly available.
- Environmental fate	and monitoring data are not available for these compounds.

- Limited information is available regarding chemical identities of commercial PFPE products (including molecular weight range, molar ratio and composition of monomer units, impurity content, functional groups) and their life cycle (including releases and degradation).

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Annex A. List of PFASs Included in the Fact Cards, Their Acronyms, CAS Registry Numbers (CASRNs), DTXSIDs and Fact Card Location

Full name	Acronym/ Trade name	CASRN	DTXSIDs ³⁹	Fact card
Phosphinic acid, <i>P</i> , <i>P</i> -bis(1,1,2,2,3,3,4,4,4- nonafluorobutyl)-; Bis(nonafluorobutyl)phosphinic acid	C ₄ /C ₄ -PFPIA / Tivida FL 2100	52299-25-9	DTXSID605 56851	#1
A mixture of perfluoroalkyl phosphonic and phosphinic acids	Masurf-780		DTXSID801 027192	#1
Phosphonic acid, perfluoro- C_{6-12} -alkyl derivs.		68412-68-0	DTXSID808 82003	#1
Phosphinic acid, bis(perfluoro- C_{6-12} -alkyl) derivs.; Phosphinic acid, bis(perfluoro- C_{6-12} -alkyl) derivatives (C_{6-12} PFPIAs)	(C ₆ –C ₁₂ PFPIAs)	68412-69-1		#1
Phosphonic acid, <i>P</i> -(1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluorohexyl)-; Perfluorohexyl phosphonic acid	C ₆ -PFPA	40143-76-8	DTXSID908 80439	#1
Phosphonic acid, <i>P</i> - (1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- heptadecafluorooctyl)-;	C ₈ -PFPA	40143-78-0	DTXSID808 79832	#1
Perfluorooctyl phosphonic acid				
Phosphonic acid, <i>P</i> - (1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heneicosafluorodecyl)-;	C ₁₀ -PFPA	52299-26-0		#1
Perfluorodecyl phosphonic acid				
Phosphinic acid, <i>P</i> - (1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- heptadecafluorooctyl)- <i>P</i> -(1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluorohexyl)-;	C ₆ /C ₈ -PFPIA	610800-34-5		#1
(Perfluorohexyl) (perfluorooctyl) phosphinic acid				
Phosphinic acid, <i>P</i> , <i>P</i> - bis(1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- heptadecafluorooctyl)-;	C ₈ /C ₈ -PFPIA	40143-79-1		#1
Bis(perfluorooctyl) phosphinic acid				
Phosphinic acid, <i>P</i> , <i>P</i> -bis(1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluorohexyl)-; Bis(perfluorohexyl) phosphinic acid	C ₆ /C ₆ -PFPIA	40143-77-9		#1
Dis(perituoronexyr) phospinine actu				

³⁹ DTXSID = Distributed Structure-Searchable Toxicity Database (DSSTox) substance ID

Phosphinic acid, <i>P</i> -(1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-	C ₆ /C ₁₀ -PFPIA	1240600-40- 1		#1
heneicosafluorodecyl)- <i>P</i> -(1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexyl)-;				
(Perfluorohexyl) (perfluorodecyl) phosphinic acid				
Phosphinic acid, <i>P</i> - (1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heneicosafluorodecyl)- <i>P</i> - (1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- heptadecafluorooctyl)-;	C ₈ /C ₁₀ -PFPIA	500776-81-8		#1
(Perfluorooctyl) (perfluorodecyl) phosphinic acid				
(Perfluorohexyl) (perfluorododecyl) phosphinic acid	C ₆ /C ₁₂ -PFPIA			#1
Octanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- pentadecafluoro-, ammonium salt (1:1); Ammonium perfluorooctanoate	APFO	3825-26-1	DTXSID803 7708	#2
Nonanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9- heptadecafluoro-, ammonium salt (1:1); Ammonium perfluorononanoate	APFN	4149-60-4	DTXSID208 80205	#2
Ammonium henicosafluoroundecanoate;	APFUnD	4234-23-5	DTXSID208 97176	#2
	ADET-D			#2
Ammonium perfluorotridecanoate	AFFIID			#2
Fatty acids Cause perfluoro ammonium salts	Surflon® S-111	72968-38-8	DTXSID801	#2
Tatty acids, C_{7-13} , permuoio, annionium sats	Summe S-111	72708-38-8	04590	π2
Acetic acid, 2,2,2-trifluoro-;	TFA	76-05-1	DTXSID904	#2
Trifluoro acetic acid			1578	
Propanoic acid, 2,2,3,3,3-pentafluoro-; Perfluoropropionic acid	PFPrA	422-64-0	DTXSID805 9970	#2
Butanoic acid, 2,2,3,3,4,4,4-heptafluoro-; Perfluorobutanoic acid; Heptafluorobutyric acid	PFBA	375-22-4	DTXSID405 9916	#2
Pentanoic acid, 2,2,3,3,4,4,5,5,5-nonafluoro-; Perfluoropentanoic acid; Perfluorovaleric acid	PFPeA	2706-90-3	DTXSID606 2599	#2
Hexanoic acid, 2,2,3,3,4,4,5,5,6,6,6-undecafluoro-;	PFHxA	307-24-4	DTXSID303	#2
Perfluorohexanoic acid			1862	
Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,7- tridecafluoro-; Perfluoroheptanoic acid	PFHpA	375-85-9	DTXSID103 7303	#2
Octanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- pentadecafluoro-; Perfluorooctanoic acid	PFOA	335-67-1	DTXSID803 1865	#2

Nonanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9- heptadecafluoro-;	PFNA	375-95-1	DTXSID803 1863	#2
Perfluorononanoic acid				
Decanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- nonadecafluoro-; Perfluorodecanoic acid	PFDA	335-76-2	DTXSID303 1860	#2
Undecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11- heneicosafluoro-; Perfluoroundecanoic acid	PFUnDA	2058-94-8	DTXSID804 7553	#2
Dodecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12- tricosafluoro-; Perfluorododecanoic acid	PFDoDA	307-55-1	DTXSID803 1861	#2
Tridecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,13-pentacosafluoro-; Perfluorotridecanoic acid	PFTrDA	72629-94-8	DTXSID908 68151	#2
Tetradecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,14,14,14-heptacosafluoro-; Perfluorotetradecanoic acid	PFTeDA	376-06-7	DTXSID305 9921	#2
Pentadecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,14,14,15,15,15-nonacosafluoro-; Perfluoropentadecanoic acid	PFPeDA	141074-63-7	DTXSID308 93341	#2
Hexadecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,14,14,15,15,16,16,16-hentriacontafluoro-; Perfluorohexadecanoic acid	PFHxDA	67905-19-5	DTXSID107 0800	#2
Heptadecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,14,14,15,15,16,16,17,17,17-tritriacontafluoro-; Perfluoroheptadecanoic acid	PFHpDA	57475-95-3	DTXSID608 96623	#2
Octadecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,14,14,15,15,16,16,17,17,18,18,18- pentatriacontafluoro-; Perfluorooctadecanoic acid	PFOcDA	16517-11-6	DTXSID106 6071	#2
Eicosanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13, 13,14,14,15,15,16,16,17,17,18,18,19,19,20,20,20- nonatriacontafluoro-; Perfluoroeicosanoic acid	PFEiDA	68310-12-3	DTXSID908 87327	#2

	1	1	1	T
1-Butanesulfonic acid, 1,1,2,2,3,3,4,4,4-nonafluoro- , potassium salt (1:1);	K-PFBS	29420-49-3	DTXSID303 7707	#3
Potassium perfluorobutanesulfonate				
1-Butanesulfonic acid, 1,1,2,2,3,3,4,4,4-nonafluoro- ; Perfluorobutanesulfonic acid	PFBS	375-73-5	DTXSID503 0030	#3
		2704.01.4		
1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5- undecafluoro-;	PFPeS	2706-91-4	DTXSID806 2600	#3
Perfluoropentanesulfonic acid				
1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluoro-; Perfluorohexanesulfonic acid	PFHxS	355-46-4	DTXSID704 0150	#3
1-Heptanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-; Perfluoroheptanesulfonic acid	PFHpS	375-92-8	DTXSID805 9920	#3
1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-; Perfluorooctanesulfonic acid	PFOS	1763-23-1	DTXSID303 1864	#3
1-Nonanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9- nonadecafluoro-;	PFNS	68259-12-1	DTXSID807 1356	#3
Pertluorononanesultonic acid				
1-Decanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heneicosafluoro-;	PFDS	335-77-3	DTXSID304 0148	#3
Perfluorodecanesultonic acid				
1-Octanesulfinic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-; Perfluorooctane sulfinic acid	PFOSI	647-29-0	DTXSID109 04262	#3
Ethanesulfonic acid, 2-[(6-chloro- 1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxy]- 1,1,2,2-tetrafluoro-, potassium salt (1:1); Potassium 9-chlorohexadecafluoro-3-oxanonane-1-	F-53B / 6:2 Cl- PFESA	73606-19-6	DTXSID608 81236	#4
sulfonate				
Propanoic acid, 2,3,3,3-tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-, ammonium salt (1:1); Hexafluoropropylene oxide-dimer acid, ammonium salt	GenX / PFPrOPrA, HFPO-DA (acid form)	62037-80-3	DTXSID401 08559	#4
Propanoic acid, 2,2,3-trifluoro-3-[1,1,2,2,3,3- hexafluoro-3-(trifluoromethoxy)propoxy]-, ammonium salt (1:1); 3H-Perfluoro-3-[(3-methoxy-propoxy)propanoic acid], ammonium salt	ADONA	958445-44-8	DTXSID008 74026	#4

Acetic acid, 2,2-difluoro-2-[[2,2,4,5-tetrafluoro-5- (trifluoromethoxy)-1,3-dioxolan-4-yl]oxy]-, ammonium salt (1:1); Perfluoro{acetic acid, 2-[(5-methoxy-1,3-dioxolan- 4-yl)oxy]}, ammonium salt	F-DIOX ammonium salt; cC6O4 ammonium salt	1190931-27- 1	DTXSID008 82626	#4
Propanoyl fluoride, 2,3,3,3-tetrafluoro-2- [1,1,2,3,3,3-hexafluoro-2-(1,1,2,2,3,3,3- heptafluoropropoxy)propoxy]-; Hexafluoropropene oxide trimer	HFPO-TA	2641-34-1	DTXSID204 4630	#4
2-(4-chloro-1,1,2,2,3,3,4,4-octafluorobutoxy)- 1,1,2,2-tetrafluoroethane-1-sulfonic acid	4:2 Cl-PFESA	737728-96-0		#4
2-[(8-Chloro-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8- hexadecafluorooctyl)oxy]-1,1,2,2- tetrafluoroethanesulfonic acid	8:2 Cl-PFESA	763051-92-9	DTXSID408 92507	#4
2-((1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxy)- 1,1,2,2-tetrafluoroethane-1-sulfonic acid	6:2 H-PFESA	874280-03-2		#4
Butanoyl fluoride, 2,2,3,3,4,4,4-heptafluoro-; Perfluorobutanoyl fluoride	PBCF	335-42-2	DTXSID004 1696	#5
Octanoyl fluoride, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- pentadecafluoro-; Perfluorooctanoyl fluoride	POCF	335-66-0	DTXSID005 9829	#5
Hexanamide, 2,2,3,3,4,4,5,5,6,6,6-undecafluoro- <i>N</i> - [3-(trimethoxysilyl)propyl]-; <i>N</i> -[3-(trimethoxysilyl)propyl]-perfluorohexanamide		154380-34-4	DTXSID808 93356	#5
Octanamide, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8- pentadecafluoro- <i>N</i> -methyl-;	MeFOA	89685-56-3	DTXSID504 78336	#5
<i>N</i> -methylperfluorooctanamide				
<i>N</i> -ethylperfluorooctanamide	EtFOA			#5
N-ethylperfluorobutanamide	EtFBA			#5
1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-; Perfluorooctanesulfonyl fluoride	POSF	307-35-7	DTXSID502 7140	#6
1-Butanesulfonyl fluoride, 1,1,2,2,3,3,4,4,4- nonafluoro-;	PBSF	375-72-4	DTXSID208 61913	#6
Perfluorobutanesulfonyl fluoride				
1-Octanesulfonamide, <i>N</i> -ethyl- 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-; <i>N</i> -Ethylperfluorooctanesulfonamide	Sulfluramid EtFOSA	4151-50-2	DTXSID103 2646	#6
Sodium 2-(<i>N</i> -ethylperfluorooctane-1- sulfonamido)ethyl phosphate; perfluorooctane sulfonamido ethanol-based phosphate diester	SAmPAP			#6
1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-; Perfluorooctanesulfonamide	FOSA	754-91-6	DTXSID303 8939	#6

1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro- <i>N</i> - methyl-;	MeFOSA	31506-32-8	DTXSID106 7629	#6
N-methyl perfluorooctane sulfonamide				
1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro- <i>N</i> - (2-hydroxyethyl)-N-methyl-;	MeFOSE	24448-09-7	DTXSID702 7831	#6
N-methyl perfluorooctane sulfonamidoethanol				
1-Octanesulfonamide, N-ethyl- 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro- <i>N</i> - (2-hydroxyethyl)-;	EtFOSE	1691-99-2	DTXSID602 7426	#6
N-ethyl perfluorooctane sulfonamidoethanol				
1-Butanesulfonamide, 1,1,2,2,3,3,4,4,4-nonafluoro- <i>N</i> -methyl-;	MeFBSA	68298-12-4	DTXSID107 1373	#6
N-methyl perfluorobutane sulfonamide				
1-Butanesulfonamide, 1,1,2,2,3,3,4,4,4-nonafluoro- <i>N</i> -(2-hydroxyethyl)- <i>N</i> -methyl-;	MeFBSE	34454-97-2	DTXSID006 7848	#6
<i>N</i> -methyl perfluorobutane sulfonamidoethanol				
1-Octanesulfonic acid, 3,3,4,4,5,5,6,6,7,7,8,8,8- tridecafluoro-;		27619-97-2	DTXSID606 7331	#7
6:2 Fluorotelomer sulfonic acid				
1-Propanaminium, <i>N</i> -(carboxymethyl)- <i>N</i> , <i>N</i> - dimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8- tridecafluorooctyl)sulfonyl]amino]-, inner salt;		34455-29-3	DTXSID404 1284	#7
6:2 Fluorotelomer sulfonamide betaine				
Silane, triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8- tridecafluorooctyl)-; Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-		51851-37-7		#7
tridecafluorooctyl)silane				
1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-;	6:2 FTOH	647-42-7	DTXSID504	#7
6:2 Fluorotelomer alcohol; 2-(perfluorohexyl)ethanol; 1 <i>H</i> ,1 <i>H</i> ,2 <i>H</i> ,2 <i>H</i> -perfluorooctan-1-ol			4572	
1-Decanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heptadecafluoro-;	8:2 FTOH	678-39-7	DTXSID702 9904	#7
8:2 Fluorotelomer alcohol;				
2-(perfluorooctyl)ethanol;				
1H,1H,2H,2H-Perfluorodecan-1-ol				
1-Dodecanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12- heneicosafluoro-;	10:2 FTOH	865-86-1	DTXSID202 9905	#7
10:2 Fluorotelomer alcohol;				
2-(perfluorodecyl)ethanol;				
1H,1H,2H,2H-perfluorododecan-1-ol				

ENV/CBC/MONO(2022)1 | 101

1-Hexanesulfonic acid, 3,3,4,4,5,5,6,6,6- nonafluoro-;	4:2 FTSA	757124-72-4	DTXSID308 91564	#7
4:2 Fluorotelomer sulfonic acid; 1 <i>H</i> ,1 <i>H</i> ,2 <i>H</i> ,2 <i>H</i> -perfluorohexanesulphonic acid				
1-Octanesulfonic acid, 3,3,4,4,5,5,6,6,7,7,8,8,8- tridecafluoro-;	6:2 FTSA	27619-97-2	DTXSID606 7331	#7
6:2 Fluorotelomer sulfonic acid; 1-Octanesulfonic acid, 3,3,4,4,5,5,6,6,7,7,8,8,8- tridecafluoro-				
1-Decanesulfonic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heptadecafluoro-;	8:2 FTSA	39108-34-4	DTXSID001 92353	#7
8:2 Fluorotelomer sulfonic acid; 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heptadecafluorodecanesulphonic acid				
1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-, 1,1'-(hydrogen phosphate);	6:2 diPAP	57677-95-9	DTXSID505 61590	#7
6:2 Fluorotelomer phosphate diester; Bis[2-(perfluorobexyl)ethyl]phosphate				
1-Decanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-	8:2 diPAP	678-41-1	DTXSID902	#7
heptadecafluoro-, 1,1'-(hydrogen phosphate);			18051	
8:2 Fluorotelomer phosphate diester; Bis[2-(perfluorooctyl)ethyl]phosphate				
1-Dodecanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12- heneicosafluoro-, 1,1'-(hydrogen phosphate);	10:2 diPAP	1895-26-7	DTXSID301 72360	#7
10:2 Fluorotelomer phosphate diester;				
Bis[2-(perfluorodecyl)ethyl]phosphate		014627 05 1		
3,3,4,4,5,5,6,6,7,7,7-Undecafluoro-2-heptanol; 5:2 fluorotelomer secondary alcohol	5:2 sFTOH (secondary alcohol, [F(CF ₂) ₅ CH(O H)CH ₃]),	914637-05-1	DTXSID805 97206	#7
4:2 Fluorotelomer unsaturated carboxylic acid	4:2 FTUCA	70887-90-0		#7
2-Octenoic acid, 3,4,4,5,5,6,6,7,7,8,8,8- dodecafluoro-;	6:2 FTUCA	70887-88-6		#7
6:2 Fluorotelomer unsaturated carboxylic acid; 2 <i>H</i> -perfluoro-2-octenoic acid				
8:2 Fluorotelomer unsaturated carboxylic acid; 2-Decenoic acid, 3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- hexadecafluoro-	8:2 FTUCA	70887-84-2	DTXSID608 25615	#7
2-Dodecenoic acid, 3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12- eicosafluoro-;	10:2 FTUCA	70887-94-4	DTXSID708 95723	#7
10:2 Fluorotelomer unsaturated carboxylic acid; 2 <i>H</i> -perfluoro-2-dodecenoic acid				

2-Propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10- heptadecafluorodecyl ester; 1 <i>H</i> ,1 <i>H</i> ,2 <i>H</i> ,2 <i>H</i> -perfluorodecyl acrylate	8:2 FTAc	27905-45-9	DTXSID506 7348	#7
1-Butanol, 2,2,3,3,4,4,4-heptafluoro-; (Perfluoropropyl)methanol	3:1 FTOH / RM 610	375-01-9	DTXSID405 9914	#8
2-Propenoic acid, 2-methyl-, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl ester, polymer with 2-propenoic acid		53515-73-4	DTXSID308 80458	#8
Oxirane, 2,2,3-trifluoro-3-(trifluoromethyl)-; Hexafluoropropylene oxide / Trifluoro(trifluoromethyl)oxirane	HFPO	428-59-1	DTXSID602 9177	#9
Furan, 2,2,3,3,4,4,5-heptafluorotetrahydro-5- (1,1,2,2,3,3,4,4,4-nonafluorobutyl)-; Perfluoro-2-butyltetrahydrofuran	FC-75	335-36-4	DTXSID608 71632	#9
Ethene, tetrafluoro-; Tetrafluoroethylene	TFE	116-14-3	DTXSID602 1325	#10
Benzenesulfonic acid, 4-[[3,4,4,4-tetrafluoro-2- [1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-1,3- bis(trifluoromethyl)-1-buten-1-yl]oxy]-, sodium salt (1:1); Sodium ρ-perfluorous nonenoxybenzene sulfonate	OBS	70829-87-7	DTXSID601 020833	#10
2-Pentenoyl fluoride, 2,3,4,5,5,5-hexafluoro-4- (trifluoromethyl)-; Perfluoro-4-methylpent-2-enoyl fluoride		88022-48-4	DTXSID408 97491	#10
2-Pentene, 1,1,2,3,4,5,5,5-octafluoro-1-iodo-4- (trifluoromethyl)-, (E)-; (2E)-1,1,2,3,4,5,5,5-Octafluoro-1-iodo-4- (trifluoromethyl)-2-pentene		120695-78-5	DTXSID206 94127	#10
1-Propene, 1,1,2,3,3,3-hexafluoro-; Hexafluoropropene	HFP	116-15-4	DTXSID202 6949	#10
Ethane, 1,1,1,2-tetrafluoro-; 1,1,1,2-Tetrafluoroethane	HFC-134a / R-134a / Freon 134a / Forane 134a / Genetron 134a / Florasol 134a / Suva 134a / Norflurane	811-97-2	DTXSID102 1324	#11
Ethene, 1,1-difluoro-; 1,1-Difluoroethylene; vinylidene fluoride	VDF	75-38-7	DTXSID302 1439	#11
1-Propene, 2,3,3,3-tetrafluoro-; 2,3,3,3-Tetrafluoropropene	HFO-1234yf	754-12-1	DTXSID407 4728	#11
Butane, 1-ethoxy-1,1,2,2,3,3,4,4,4-nonafluoro-; Ethylnonafluorobutylether	HFE-7200	163702-05-4	DTXSID007 3118	#11

ENV/CBC/MONO(2022)1 | 103

Methane, (difluoromethoxy)trifluoro-;	HFE-125	3822-68-2	DTXSID407 3968	#11
Propane, 1,1,1,2,3,3,3-heptafluoro-; 1,1,1,2,3,3,3-heptafluoropropane	HFC-227ea	431-89-0		#11
Propane, 1,1,1,3,3,3-hexafluoro-; 1,1,1,3,3,3-hexafluoropropane	HFC-236fa	690-39-1	DTXSID805 2435	#11
2-Butene, 1,1,1,4,4,4-hexafluoro-, (2Z)-; (Z)-1,1,1,4,4,4-hexafluorobut-2-ene	HFO-1336mzz	692-49-9	DTXSID008 83476	#11
Ethane, 1,1,1,2,2-pentafluoro-; 1,1,1,2,2-pentafluoroethane	HFC-125	354-33-6	DTXSID102 4251	#11
Propane, 1,1,1,3,3-pentafluoro-; 1,1,1,3,3-pentafluoropropane	HFC-245fa	460-73-1	DTXSID605 2110	#11
Butane, 1,1,1,3,3-pentafluoro-; 1,1,1,3,3-pentafluorobutane	HFC-365mfc	406-58-6	DTXSID507 3901	#11
Pentane, 1,1,1,2,2,3,4,5,5,5-decafluoro-; 1,1,1,2,2,3,4,5,5,5-decafluoropentane	HFC-43-10mee	138495-42-8	DTXSID308 69884	#11
1-Propene, 1,3,3,3-tetrafluoro-, (1E)-; 1,3,3,3-tetrafluoroprop-1-ene	HFC-1234ze	29118-24-9	DTXSID609 36952	#11
Benzene, (trifluoromethyl)-; Benzotrifluoride		98-08-8	DTXSID202 4589	#12
Benzene, 1-chloro-4-(trifluoromethyl)-; 1-Chloro-4-(trifluoromethyl)benzene		98-56-6	DTXSID702 4821	#12
Benzenepropanamine, <i>N</i> -methyl-γ-[4- (trifluoromethyl)phenoxy]-	Fluoxetine	54910-89-3	DTXSID702 3067	#12
Urea, <i>N</i> , <i>N</i> -dimethyl- <i>N</i> '-[3-(trifluoromethyl)phenyl]-	Fluometuron	2164-17-2	DTXSID802 0628	#12
Ethene, 1,1,2,2-tetrafluoro-, homopolymer; Polytetrafluoroethylene	PTFE	9002-84-0	DTXSID704 7724	#13
Ethene, 1,1-difluoro-, homopolymer; Polyvinylidene fluoride	PVDF	24937-79-9	DTXSID808 95097	#13
1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1,2,2-tetrafluoroethene; Fluorinated ethylene propylene	FEP	25067-11-2	DTXSID708 80371	#13
Propane, 1,1,1,2,2,3,3-heptafluoro-3-[(1,2,2- trifluoroethenyl)oxy]-, polymer with 1,1,2,2- tetrafluoroethene; Perfluoro-3-[(trifluoroethenyl)oxy]propane, polymer with tetrafluoroethene		26655-00-5	DTXSID408 80383	#13
Ethene, 1,1,2,2-tetrafluoro-, polymer with 1,1,2- trifluoro-2-(1,1,2,2,2-pentafluoroethoxy)ethane; Tetrafluoroethene polymer with trifluoro(pentaflurorethoxy)ethene		31784-04-0	DTXSID108 81948	#13

1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with1,1-difluoroethene;1,1-Difluorethylene-hexafluorpropene polymer	9011-17-0	DTXSID308 80211	#14
1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1,1,2,2,3,3-heptafluoro-3-[(1,2,2- trifluoroethenyl)oxy]propane and 1,1,2,2- tetrafluoroethene; Hexafluoropropene, 1-((trifluoroethenyl)oxy)hepta- fluoropropane, tetrafluoroethene polymer	63654-41-1	DTXSID108 80532	#14