

1 Introduction

This fact sheet addresses naming conventions of some of the most commonly reported PFAS considering historical use, current state of science research related to environmental occurrence, and available commercial analyses. For naming conventions related to additional PFAS, refer to Buck et al. (2011).

The PFAS family may be divided into two primary classes: polymer and nonpolymer as shown in Figure 1. Future updates to the family tree and nomenclature are expected given the evolving public knowledge of these compounds.

This fact sheet focuses primarily on nonpolymer PFAS most commonly detected in the environment. Additional information is available in the Guidance Document.

2 Nonpolymer PFAS

The class of nonpolymer PFAS encompasses two major subclasses: perfluoroalkyl substances and polyfluoroalkyl substances, which include many groups and subgroups of chemicals, examples of which are shown in Figure 1. These compounds were selected as the focus of the Guidance Document because they (1) are most commonly detected (to date) in humans, biota, and other environmental media; (2) appear to be relatively more abundant at PFAS investigation sites; (3) may have data available regarding potential human health and ecological effects from environmental exposure; (4) may have state or federal guidance values; and/or (5) are included in most laboratory PFAS analyte lists.

ITRC has developed a series of fact sheets that summarize recent science and emerging technologies regarding PFAS. The information in this and other PFAS fact sheets is more fully described in the **ITRC PFAS Technical and Regulatory Guidance Document (Guidance Document)** (<https://pfas-1.itrcweb.org/>).

This fact sheet describes methods for classifying PFAS that may be found in the environment, including:

- Polymer and Nonpolymer PFAS
- Perfluoroalkyl acids
- Long- and Short-Chain PFAS
- Polyfluoroalkyl substances
- Linear vs. Branched PFAS
- Acids vs. Anions
- Replacement PFAS Chemistry

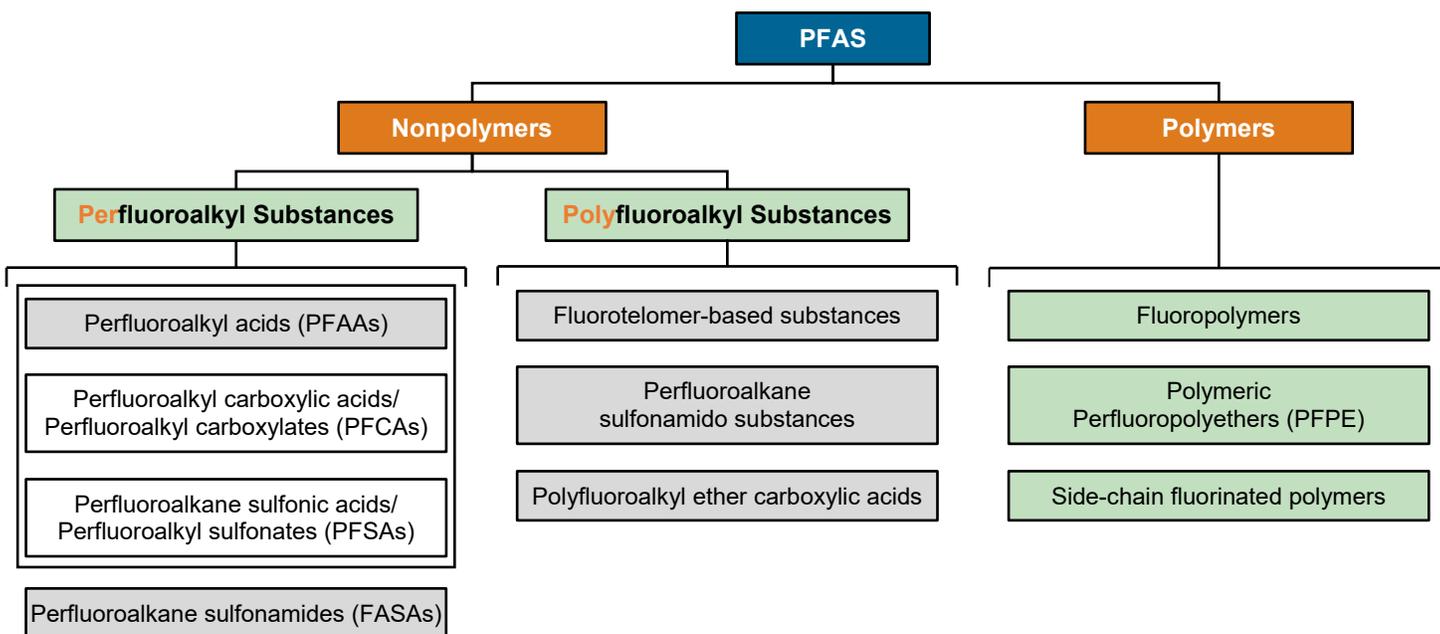


Figure 1. Summary of the PFAS family.

Naming Conventions for Per- and Polyfluoroalkyl Substances (PFAS) *continued*

Perfluoroalkyl Substances

Perfluoroalkyl substances are fully fluorinated (perfluoro-) alkane (carbon-chain) molecules. Their basic chemical structure is a chain (or tail) of two or more carbon atoms with a charged functional group (or head) attached at one end. The functional groups commonly are carboxylates or sulfonates, but other forms are also detected in the environment. This structure, which is illustrated in Figure 2 for perfluorooctane *sulfonate* (PFOS) and perfluorooctane *carboxylate*, referred to as perfluorooctanoate (PFOA), can be written as:

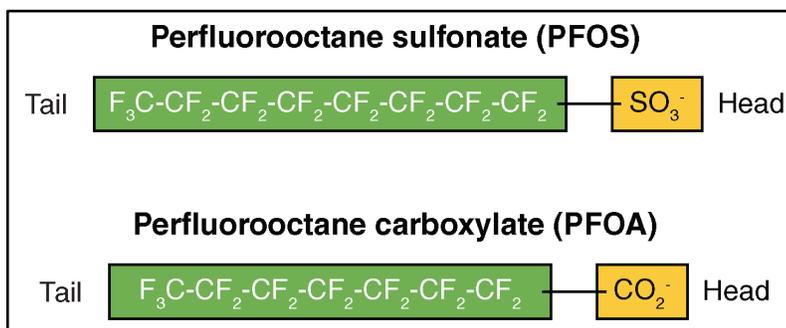


Figure 2. The head and tail structure of PFOS and PFOA.

$\text{C}_n\text{F}_{2n+1}\text{-R}$

where “ $\text{C}_n\text{F}_{2n+1}$ ” defines the length of the perfluoroalkyl chain tail, “n” is ≥ 2 , and “R” represents the attached functional group head. The functional group may contain 1 or more carbon atoms, which are included in the total number of carbons when naming the compound.

Perfluoroalkyl acids (PFAAs)

Perfluoroalkyl acids (PFAAs) are some of the least complex PFAS and currently are the class of PFAS most commonly tested for in the environment. Biotic and abiotic degradation of many polyfluoroalkyl substances may result in the formation of PFAAs. As a result, PFAAs are sometimes referred to as “terminal PFAS” or “terminal degradation products,” meaning no further degradation products will form from them under normal environmental conditions. Polyfluoroalkyl PFAS that degrade to create PFAAs are referred to as “precursors.” PFAAs are divided into two major subgroups:

- *Perfluoroalkyl carboxylic acids* (PFCAs), or perfluoroalkyl carboxylates, are terminal degradation products of select precursor polyfluoroalkyl substances, such as fluorotelomer alcohols (FTOHs). An example PFCa is PFOA.
- *Perfluoroalkane sulfonic acids* (PFSAs), or perfluoroalkyl sulfonates, are also terminal degradation products of select precursor polyfluoroalkyl substances, such as perfluoroalkyl sulfonamido ethanols (FASEs). An example PFSA is PFOS.

Many of the commonly detected PFAAs are denoted using the structural shorthand:

PFXY

where:

PF = perfluoro

X = the carbon chain length using the same naming conventions as hydrocarbons based on the number of carbons (*for example, B for butane or 4 carbons, Pe for pentane or 5 carbons*)

Y = the functional group (*for example, A = carboxylate or carboxylic acid and S = sulfonate or sulfonic acid*)

PFAAs are the majority of PFAS typically included in commercial laboratory target analyte lists and are the primary PFAS for which federal or state health-based guidance values have been established. As a result, PFAAs tend to drive site investigation and remediation decisions, and so it is helpful to understand the naming conventions for this class.

Table 1 illustrates how this naming structure works for select PFCAs and PFSAs, which collectively are referred to as PFAAs. The full table is included in the Guidance Document.

Table 1. Basic naming structure and shorthand for select PFAAs

X	Y	Acronym	Name	Formula	CAS No.
B = buta (4 carbon)	A = Carboxylate or carboxylic acid	PFBA	Perfluorobutanoate	$\text{C}_3\text{F}_7\text{CO}_2^-$	45048-62-2
			Perfluorobutanoic acid	$\text{C}_3\text{F}_7\text{COOH}$	375-22-4
	S = Sulfonate or sulfonic acid	PFBS	Perfluorobutane sulfonate	$\text{C}_4\text{F}_9\text{SO}_3^-$	45187-15-3
			Perfluorobutane sulfonic acid	$\text{C}_4\text{F}_9\text{SO}_3\text{H}$	375-73-5
O = octa (8 carbon)	A = Carboxylate or carboxylic acid	PFOA	Perfluorooctanoate	$\text{C}_7\text{F}_{15}\text{CO}_2^-$	45285-51-6
			Perfluorooctanoic acid	$\text{C}_7\text{F}_{15}\text{COOH}$	335-67-1
	S = Sulfonate or sulfonic acid	PFOS	Perfluorooctane sulfonate	$\text{C}_8\text{F}_{17}\text{SO}_3^-$	45298-90-6
			Perfluorooctane sulfonic acid	$\text{C}_8\text{F}_{17}\text{SO}_3\text{H}$	1763-23-1

Naming Conventions for Per- and Polyfluoroalkyl Substances (PFAS) *continued*

Long-Chain versus Short-Chain Distinction

PFAAs are sometimes described as long-chain and short-chain to group PFCAs and PFSAAs that may behave similarly in the environment. Table 2 illustrates the differences in the short-chain and long-chain PFCAs and PFSAs.

Table 2. Short-chain and long-chain PFCAs and PFSAs

Number of Carbons	4	5	6	7	8	9	10	11	12
PFCAs	Short-chain PFCAs				Long-chain PFCAs				
	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA
PFSAs	PFBS	PFPeS	PFHxS	PFHpS	PFOS	PFNS	PFDS	PFUnS	PFDoS
	Short-chain PFSAs		Long-chain PFSAs						

Anion versus Acid Form

As noted above, the names for the anionic and acid forms of PFAAs are often used interchangeably. However, it is critical to know which form is being discussed because of differences in their physical and chemical properties and behavior in the environment. Some important things to keep in mind regarding the anionic vs. acid forms are:

- Most PFAAs are present in environmental and human matrices in their anionic form. For example, PFOS is present in the environment in the anionic form, perfluorooctane sulfonate.
- Although laboratories may be reporting PFOA or PFOS using the acid form of their name, they are actually measuring the anionic form (for example, octanoate or sulfonate), as this is the form that exists in the environment.
- The acid form and their associated cationic salts have CAS numbers, while the anionic forms may not. For example, PFOS can exist as different salts (cationic), including sodium, lithium, potassium, or ammonium. Each of these salts will have a different CAS number:
- When the salt or acid exists in water or other liquids, it will dissociate (lose its hydrogen) and the salt or acid will break off and form the anion (for example, COO⁻).

Linear and Branched Isomers of PFAS

Many PFAS may be present as mixtures of linear and branched isomers (chemicals with the same chemical formula, but different molecular structures) depending on the manufacturing process that was used. These structural differences are important because they may affect how the compounds behave in the environment. The presence of linear and branched isomers may be useful in understanding sources of PFAS and the age of the source, since the production of isomers varies by manufacturing processes. For example, the fluorotelomerization process produces primarily linear PFAAs, whereas the ECF process produces a mixture of linear and branched PFAA isomers. The presence of linear and branched isomers may also have implications for partitioning, transport, and bioaccumulation.

Polyfluoroalkyl Substances

Polyfluoroalkyl substances and some side-chain fluorinated polymers are increasingly being identified as important to understanding the fate and transport of PFAS at release sites and in the environment (OECD 2013; Butt, Muir, and Mabury 2014; Liu and Mejia-Avendaño 2013; Wang et al. 2011; Mejia-Avendaño et al. 2016). Figure 1 highlights the polyfluoroalkyl substances that, to date, have most commonly been detected at PFAS sites (Barzen-Hanson et al. 2017).

Polyfluoroalkyl substances are distinguished from perfluoroalkyl substances by not being fully fluorinated. Instead, they have a non-fluorine atom (typically hydrogen or oxygen) attached to at least one, but not all, carbon atoms, while at least two or more of the remaining carbon atoms in the carbon chain tail are fully fluorinated. Figure 3 shows an example of a polyfluoroalkyl substance where two of the carbons in the tail are not fully fluorinated, while the remaining carbons are. This also illustrates the “n:x” naming convention where “n” is the number of fully fluorinated carbons (in this case, 8) and “x” is the number of carbons that are not fully fluorinated (in this case, 2).

The carbon-hydrogen (or other non-fluorinated) bond in polyfluoroalkyl molecules creates a “weak” point in the carbon chain that is susceptible to biotic or abiotic degradation. As a result, many polyfluoroalkyl substances that contain a perfluoroalkyl CF group are potential precursor compounds that have the potential to be transformed into PFAAs.

Naming Conventions for Per- and Polyfluoroalkyl Substances (PFAS) *continued*

Fluorotelomer Substances

Fluorotelomer substances are polyfluoroalkyl substances produced by the fluorotelomerization process. The degradation of fluorotelomer-based substances is a potential source of PFCAs in the environment, but not PFSA (Buck et al. 2011). The following fluorotelomer substances are those most commonly detected in the environment to date:

- Fluorotelomer alcohols (FTOH): The n:2 fluorotelomer alcohols (n:2 FTOHs) are key raw materials in the production of n:2 fluorotelomer acrylates and n:2 fluorotelomer methacrylates (Buck et al. 2011).
- Fluorotelomer sulfonic acids (FTSA): The n:2 fluorotelomer sulfonic acids (n:2 FTSA) have been detected in environmental matrices at sites where aqueous film forming foam (AFFF) has been used, and also in wastewater treatment plant effluents and landfill leachate. FTSA are precursor compounds and can undergo aerobic biotransformation to form PFCAs (Buck et al. 2011).
- Fluorotelomer carboxylic acids (FTCA): These compounds form through the biodegradation of FTOHs (Buck et al. 2011; Liu and Mejia Avendaño 2013) and have been detected in landfill leachate.

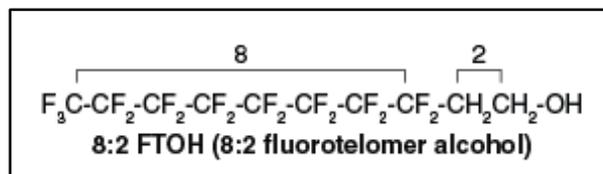


Figure 3. Example of a polyfluoroalkyl substance.

3 Polymer PFAS

Polymers are large molecules formed by combining many identical smaller molecules (or monomers) in a repeating pattern. Polymer substances in the PFAS family include fluoropolymers, polymeric perfluoropolyethers (polymeric PFPE), and side-chain fluorinated polymers. In general, some polymer PFAS are currently believed to pose less immediate human health and ecological risk relative to some nonpolymer PFAS. As stated previously, most compounds of interest at environmental release sites are nonpolymers.

4 Replacement Chemistry

Concern regarding the persistence, bioaccumulation, and possible ecological and human health effects of long-chain PFAAs has led manufacturers to develop replacement short-chain PFAS that should not degrade to long-chain PFAAs (USEPA 2006a; OECD 2017). The short-chain alternatives include, but are not limited to, fluorotelomer-based products with a six-carbon perfluorohexyl chain and ECF-based products with a four-carbon perfluorobutyl chain. These products may degrade to form short-chain PFAAs, such as PFHxA and PFBS, respectively (Wang, Cousins, et al. 2013; Buck 2015). While a full discussion of replacement chemistries is not possible here, it is important to be aware of this trend toward shorter-chain chemistries, as some of these PFAS increasingly may be detected in the environment. With the 2015 major global manufacturers' phase-out of certain long-chain PFAAs and their potential precursors (for example, PFOA and 8:2 FTOH) replacement PFAS have been commercially introduced (many following review by USEPA) and may continue to be developed. Several studies suggest some alternate PFAS may or may not be less hazardous than the long-chain predecessors, although publicly available information on most replacement chemicals is limited (Wang, Cousins, et al. 2015; RIVM 2016; OECD 2015b).

5 References and Acronyms

The references cited in this fact sheet and further references can be found at <https://pfas-1.itrcweb.org/references/>. The acronyms used in this fact sheet and in the Guidance Document can be found at <https://pfas-1.itrcweb.org/acronyms/>.



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