

1 Introduction

The following topics are covered in this fact sheet:

- Polymer vs. Nonpolymer PFAS
- Perfluoroalkyl substances
- Polyfluoroalkyl substances
- PFAA Naming Conventions
- Long-Chain vs. Short-Chain
- Linear vs. Branched
- Acid vs. Anion
- Replacement Chemistry
- Physical and Chemical Properties

This fact sheet uses three conventions worth highlighting:

- **Anionic form of chemical names:** Many PFAS can exist in various ionic states (for example, acids, anions, cations), which has important implications for their chemical and physical properties. In most cases, this fact sheet uses the anionic form of a given PFAS name, as this is the state in which most PFAS exist in the environment.
- **“PFC” is not used:** The acronym “PFC” is poorly defined in the scientific literature, but typically refers to “**per**fluorinated compounds.” It does not include polyfluorinated substances which are increasingly recognized as important contaminants at many PFAS sites, while it does include unrelated chemicals that are not of concern at those sites.
- **“PFAS”, not “PFASs”:** The acronym “PFAS” stands for “per- **and** polyfluoroalkyl substances.” No single chemical within the PFAS class can be both polyfluorinated and perfluorinated, so by definition “PFAS” is plural and a small “s” is not needed. Some authors elect to add a small “s” to this acronym (PFASs) to emphasize the fact that it is plural, but it is not needed. When referring to a single chemical within the PFAS class, it is usually more accurate to simply name that specific chemical.

USEPA has compiled an online resource for PFAS information. The information includes topics such as Policy and Guidance, Chemistry and Behavior, Occurrence, Toxicology, Site Characterization and Remediation Technologies (USEPA 2017h).

1.1 Why do we need to understand PFAS Naming Conventions?

The number and complexity of environmentally-relevant PFAS and the exponential increase in related scientific publications have led to confusion in the environmental community and the public (Buck et al. 2011; Wang et al. 2017). The use of non-specific acronyms, such as perfluorinated compound (PFC), has hampered clarity of investigative results. Use of consistent naming conventions by researchers, practitioners, regulators, and stakeholders will reduce confusion and support clearer communication.

Proper naming also helps to distinguish PFAS from other organic compounds that contain fluorine. PFAS, which are fluorinated aliphatic (carbon chain) substances, do not include aromatic (carbon ring) substances that contain carbon-fluorine (C-F) bonds (for example, active pharmaceutical ingredients, crop protection) or chlorofluorocarbons (refrigerants). This is another reason to avoid the use of the more generic acronym, PFC, which can include these non-PFAS.

Chemical Abstract Service (CAS) numbers are another helpful tool for clearly identifying the chemical that is being referenced. However, even these have led to confusion when it comes to PFAS. Some PFAS may occur in various ionic states, such as acids, anions (negatively charged), cations (positively charged salts), and zwitterions (both positively and negatively charged dipolar molecules), each of which has its own CAS number (and some have no CAS number). The ionic state determines its electrical charge and its physical and chemical properties, which in turn controls its fate and

ITRC has developed a series of six fact sheets to summarize the latest science and emerging technologies regarding PFAS. The purpose of this fact sheet is to:

- Provide an overview of terminology, names, and acronyms for PFAS, focusing on those most commonly reported in the environment. The fact sheet focuses on those PFAS most commonly tested for by current analytical methods, but also describes other important classes of PFAS.
- Summarize the common physical and chemical properties associated with PFAS, along with a discussion of those properties for which no data are currently available.

For further information, please see the ITRC Technical and Regulatory Guidance document for PFAS dated April 2020.

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

transport in the environment and potential human health and ecological effects. Chemical and physical properties of the various states of a given per- or polyfluoroalkyl substance can be so different that they completely alter critical aspects of the substance, such as solubility, volatility, and bioaccumulative potential. As a result, care must be taken in selecting the correct CAS number to avoid confusion regarding the chemistry and behavior of the chemical being described.

2 PFAS Families

PFAS encompass a wide universe of substances with very different physical and chemical properties, including gases (for example, perfluorobutane), liquids (for example, fluorotelomer alcohols), surfactants (for example, perfluorooctane sulfonate), and solid material high-molecular weight polymers (for example, polytetrafluoroethylene [PTFE]). For this reason, it is helpful to arrange PFAS that share similar chemical and physical properties into families.

The PFAS families may be divided into two primary categories: polymer and nonpolymer as shown in Figure 2-1. This fact sheet focuses primarily on nonpolymer PFAS most commonly detected in the environment. The polymer family of PFAS is not addressed in detail in this fact sheet. Buck et al. (2011) is an open-access paper that provides a more detailed explanation of PFAS terminology, classification, and origins, and recommends specific and descriptive terminology, names, and acronyms for PFAS.

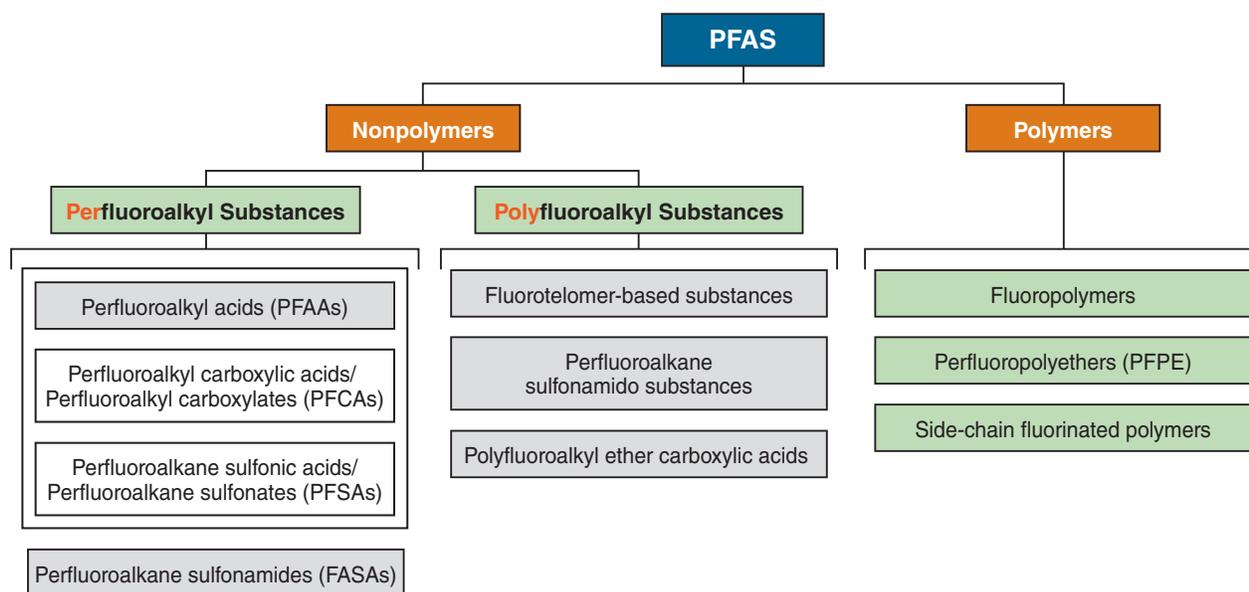


Figure 2-1. Summary of PFAS families

2.1 Nonpolymer PFAS

The family of nonpolymeric PFAS encompasses two major classes: perfluoroalkyl substances and polyfluoroalkyl substances, which include many subgroups of chemicals, examples of which are shown in Figure 2-1. Table 2-1 provides general classification and chemical structures, examples of each class, and primary uses of the nonpolymer PFAS highlighted in Figure 2-1. These compounds were selected as the focus of this fact sheet because they (1) are most commonly detected in humans, biota, and other environmental media; (2) appear to be relatively more abundant at PFAS investigation sites; (3) may have state or federal guidance values (see the *Regulations, Guidance, and Advisories Fact Sheet*); and/or (4) are included in most laboratory PFAS analyte lists.

2.1.1 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 *head* attached at one end. The functional groups commonly are carboxylates or sulfonates, but other forms are also detected in the environment. Fluorine atoms are attached to all possible bonding sites along the carbon chain of the tail, except for one bonding site on the last carbon where the functional group head is attached. This structure, which is illustrated in Figure 2-2 for perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA), can be written as:



Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

where “C_nF_{2n+1}” defines the length of the perfluoroalkyl chain tail, “n” is >2, and “R” represents the attached functional group head. Note that the functional group may contain 1 or more carbon atoms, which are included in the total number of carbons when naming the compound.

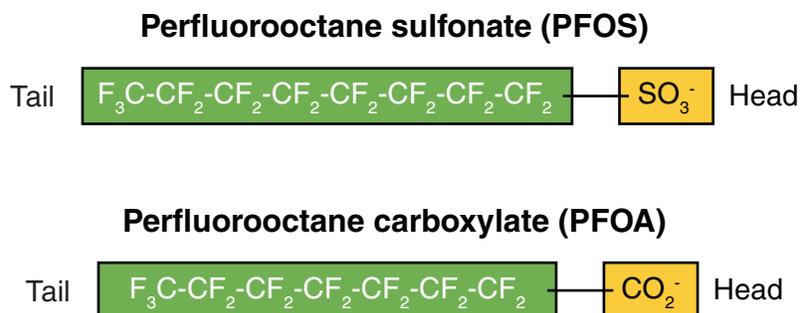


Figure 2-2. The tail and head structure of PFOS and PFOA molecules

Table 2-1. Major PFAS classes discussed in this fact sheet

Source: Adapted with permission from Buck, R.C., J. Franklin, U. Berger, J. M. Conder, I. T. Cousins, P. de Voogt, A. A. Jensen, K. Kannan, S. A. Mabury, and S. P. van Leeuwenet. 2011. “Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification, and Origins.” *Integrated Environmental Assessment and Management*, 7:513-541. Open access. Copyright 2011 SETAC. <http://dx.doi.org/10.1002/ieam.258>

Family	Class	Group	General Chemical Structure: C _n F _{2n+1} R, where R =	Examples	Uses
PERFLUORINATED	Perfluoroalkyl acids (PFAAs)	Perfluoroalkyl carboxylic acids (PFCAs)	-COOH	Perfluorooctanoic acid (PFOA), C ₇ F ₁₅ COOH	Surfactant
		Perfluoroalkyl carboxylates (PFCAs)	-COO ⁻	Perfluorooctanoate (PFOA), C ₇ F ₁₅ COO ⁻	
		Perfluoroalkane sulfonic acids (PFSAAs)	-SO ₃ H	Perfluorooctane sulfonic acid (PFOS), C ₈ F ₁₇ SO ₃ H	Surfactant
		Perfluoroalkane sulfonates (PFSAAs)	-SO ₃ ⁻	Perfluorooctane sulfonate (PFOS), C ₈ F ₁₇ SO ₃ ⁻	
	Perfluoroalkane sulfonamides (FASAs)	Perfluoroalkane sulfonamides (FASAs)	-SO ₂ NH ₂	Perfluorooctane sulfonamide (FOSA), C ₈ F ₁₇ SO ₂ NH ₂	Major raw material for surfactant and surface protection products

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

Family	Class	Group	General Chemical Structure: $C_nF_{2n+1}R$, where $R =$	Examples	Uses
POLYFLUORINATED	Fluorotelomer substances	n:2 Fluorotelomer alcohols (n:2 FTOHs)	-CH ₂ CH ₂ OH	10:2 Fluorotelomer alcohol (10:2 FTOH), C ₁₀ F ₂₁ CH ₂ CH ₂ OH	Major raw material for surfactant and surface protection products
		n:2 Fluorotelomer sulfonic acids (n:2 FTSAAs)	-CH ₂ CH ₂ SO ₃ H	8:2 Fluorotelomer sulfonic acid (8:2 FTSA), C ₈ F ₁₇ CH ₂ CH ₂ SO ₃ H	Surfactant and environmental transformation products
		Fluorotelomer carboxylic acids (FTCAs)	-CH ₂ COOH	6:2 Fluorotelomer carboxylic acid (6:2 FTCA), C ₆ F ₁₃ CH ₂ COOH	Intermediate environmental transformation product
			-CH ₂ CH ₂ COOH	5:3 Fluorotelomer carboxylic acid (5:3 Acid), C ₅ F ₁₁ CH ₂ CH ₂ COOH	
	Perfluoroalkane sulfonamido substances	N-alkyl perfluoroalkane sulfonamides (N-alkyl FASAs) (MeFASAs, EtFASAs, BuFASAs)	-SO ₂ N(R')H where R' = C _m H _{2m+1} (m = 1, 2, 4)	N-Ethyl perfluorooctane sulfonamide (EtFOSA), C ₈ F ₁₇ SO ₂ N(C ₂ H ₅)H	Major raw material for surfactant and surface protection products
				N-Methyl perfluorooctane sulfonamide (MeFOSA), C ₈ F ₁₇ SO ₂ N(CH ₃)H	
		Perfluoroalkane sulfonamido ethanols (FASEs) and N-alkyl perfluoroalkane sulfonamido ethanols (MeFASEs, EtFASEs, BuFASEs)	SO ₂ N(R')CH ₂ CH ₂ OH where R' = C _m H _{2m+1} (m = 0, 1, 2, 4)	N-Ethyl perfluorooctane sulfonamidoethanol (EtFOSE), C ₈ F ₁₇ SO ₂ N(C ₂ H ₅)CH ₂ CH ₂ OH	Major raw material for surfactant and surface protection products
				N-Methyl perfluorooctane sulfonamido ethanol (MeFOSE), C ₈ F ₁₇ SO ₂ N(CH ₃)CH ₂ CH ₂ OH	
		Perfluoroalkane sulfonamido acetic acids (FASAAs) and N-alkyl perfluoroalkane sulfonamido acetic acids (MeFASAAs, EtFASAAs, BuFASAAs)	SO ₂ N(R')CH ₂ COOH where R' = C _m H _{2m+1} (m = 0, 1, 2, 4)	N-Ethyl perfluorooctane sulfonamido acetic acid (EtFOSAA), C ₈ F ₁₇ SO ₂ N(C ₂ H ₅)CH ₂ CO ₂ H	Intermediate environmental transformation product
				N-Methyl perfluorooctane sulfonamido acetic acid (MeFOSAA), C ₈ F ₁₇ SO ₂ N(CH ₃)CH ₂ CO ₂ H	

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

2.1.1.1 Perfluoroalkyl acids (PFAAs)

Perfluoroalkyl acids (PFAAs) are some of the most basic PFAS molecules. They are essentially non-degradable 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 environmental conditions. Polyfluoroalkyl substances that degrade to create terminal PFAAs are referred to as “precursors.” The PFAA class is divided into two major groups (also shown in Table 2-1):

- *Perfluoroalkyl carboxylic acids* (PFCAs), or perfluoroalkyl carboxylates, are terminal degradation products of select precursor polyfluoroalkyl substances, such as fluorotelomer alcohols (FTOHs). The most frequently detected PFCA is PFOA.
- *Perfluoroalkane sulfonic acids* (PFSAs), or perfluoroalkyl sulfonates, are also terminal degradation products of select precursor polyfluoroalkyl substances, such as perfluoroalkyl sulfonamidoethanols (FASEs). The most frequently detected PFSA is PFOS.

2.1.1.2 Perfluoroalkane sulfonamides (FASAs)

Perfluoroalkane sulfonamides (FASAs), such as perfluorooctane sulfonamide (FOSA), are used as raw material to make perfluoroalkyl sulfonamide substances that are used for surfactants and surface treatments. FASAs can degrade to form PFAAs such as PFOS.

2.1.2 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 2-1 highlights the polyfluoroalkyl substances that, to date, have most commonly been detected at PFAS sites (see 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 2-3).

Fluorotelomer-based polyfluoroalkyl substances are named using an “n:x” prefix where “n” indicates the number of fully fluorinated carbon atoms ($n > 2$) and “x” indicates the number of carbon atoms that are not fully fluorinated ($x > 1$). An example of a polyfluoroalkyl substance is shown in Figure 2-3, which also illustrates the “n:x” naming convention.

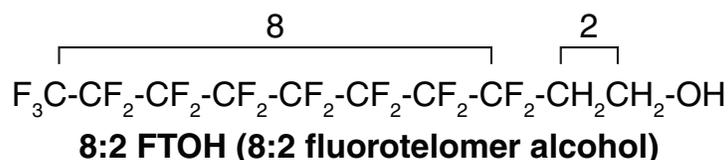


Figure 2-3. Example of a polyfluoroalkyl substance where two of the carbons in the tail are not fully fluorinated, while the remaining carbons are. This also illustrates the “n:x” naming convention where “n” is the number of fully fluorinated carbons (in this case, 8) and “x” is the number of carbons 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 $\text{C}_n\text{F}_{2n+1}$ group are potential precursor compounds that have the potential to be transformed into PFAAs.

Figures 2-4 and 2-5 provide some examples of degradation pathways for environmentally relevant polyfluoroalkyl precursors derived from two PFAS production methods, telomerization and electrochemical fluorination (ECF), respectively. Note that these figures include some PFAS not discussed in this fact sheet, but described in Buck et al. (2011).

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

2.1.2.1 Fluorotelomer Substances

Fluorotelomer substances are polyfluoroalkyl substances produced by the fluorotelomerization process. As shown in Figure 2-4, the degradation of fluorotelomer-based substances is a potential source of PFCAs in the environment, but not PFSAAs (Buck et al. 2011). For many of these compounds, the naming convention identifies the number of fully fluorinated carbon atoms and the number of carbon atoms that are not fully fluorinated.

Fluorotelomer Degradation Pathway Overview

Example for 8:2 fluorotelomer homologue

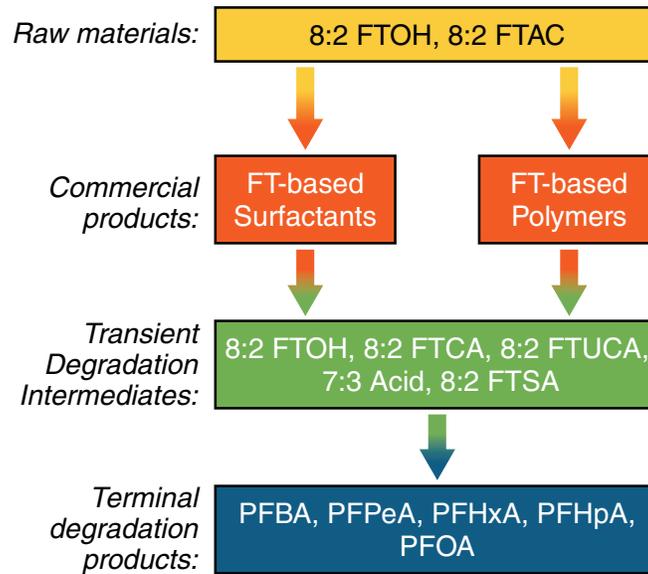


Figure 2-4. Fluorotelomer degradation pathway overview (Example for 8:2 fluorotelomer homologue)

ECF Degradation Pathway Overview

Example for perfluorooctane sulfonyl homologue

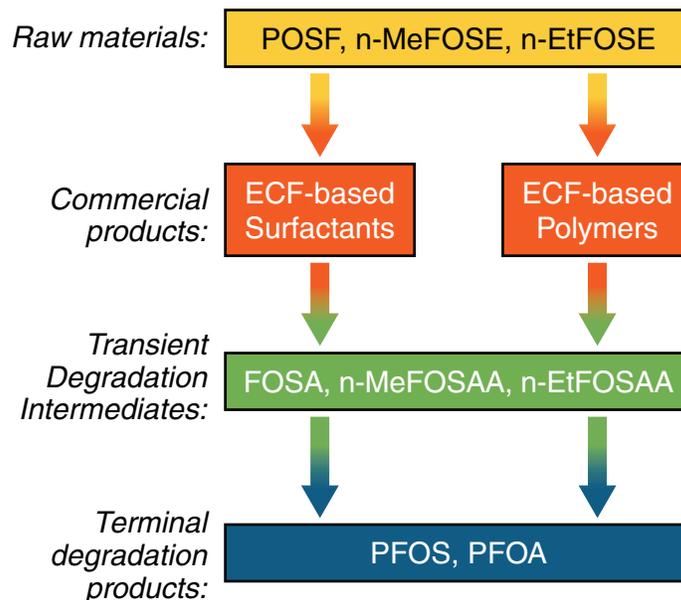


Figure 2-5. ECF degradation pathway overview (Example for perfluorooctane sulfonyl homologue).

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

The following fluorotelomer substances (also shown in Table 2-1) 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 (Figure 2-3; Buck et al. 2011; Liu and Mejia Avendaño 2013) and have been detected in landfill leachate. Note that the –COOH functional group on these fluorotelomer compounds mean they may have either an even or odd number of carbons, so they may have n:2 or n:3 prefixes.

2.1.2.2 Perfluoroalkane Sulfonamido Substances

All of the families of perfluoroalkane sulfonamido substances shown in Table 2-1 and discussed below have been detected in the environment and humans. *Perfluoroalkane* refers to the fully fluorinated carbon chain tail, but these compounds also contain one or more CH₂ groups in the head of the molecule attached to the sulfonamido spacer (see Figure 2-6). They are either used as raw materials for surfactant and surface treatment products, or they are present as intermediate transformation products of these raw materials. As shown in Figure 2-5, some perfluoroalkane sulfonamido substances have been found to degrade to PFOS (Mejia Avendaño and Liu 2015). Environmentally relevant perfluoroalkane sulfonamido substances include:

- *Perfluoroalkane sulfonamido ethanols* (FASEs) and *N-alkyl perfluoroalkane sulfonamido ethanols* (MeFASEs, EtFASEs, BuFASEs) are raw materials for surfactant and surface treatment products (Buck et al. 2011). Figure 2-6 illustrates the structure of N-EtFOSE.
- *Perfluoroalkane sulfonamido acetic acids* (FASAAs) and *N-alkyl perfluoroalkane sulfonamido acetic acids* (MeFASAAs, EtFASAAs, BuFASAAs) are intermediate transformation products of FASEs, MeFASEs, EtFASEs, and BuFASEs (see Figure 2-5) (Buck et al. 2011).
- *N-alkyl perfluoroalkane sulfonamides* (*N-alkyl FASAs*) are transformation products that include N-Methyl perfluorooctane sulfonamide (MeFOSA) and N-Ethyl perfluorooctane sulfonamide (EtFOSA).

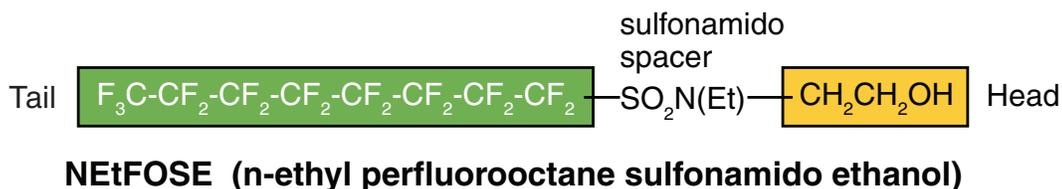


Figure 2-6. Example perfluoroalkane sulfonamido ethanol (FASE)

2.2 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, perfluoropolyethers (PFPE), and side-chain fluorinated polymers.

Side-chain fluorinated polymers contain a nonfluorinated polymer backbone from which fluorinated side chains branch off. Some may become precursors for PFAAs when the point of connection of a fluorinated side-chain on a polymer is broken to release a PFAA.

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.

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

3 PFAA Naming Conventions

PFAAs are the group of PFAS that make up 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, they tend to drive site investigation and remediation decisions, and so it is helpful to understand the naming conventions for this class. Many of the commonly detected PFAAs are denoted using the structural shorthand:

PFX_Y

where:

PF = perfluoroalkyl

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

Table 3-1 illustrates how this naming structure works for the PFCAs and PFSAs, which collectively are referred to as PFAAs.

Table 3-1. Basic naming structure and shorthand for perfluoroalkyl acids (PFAAs)

X	Y	Acronym	Name	Formula	CAS No.
B = buta (4 carbon)	A = Carboxylate or carboxylic acid	PFBA	Perfluorobutanoate	$C_3F_7CO_2^-$	45048-62-2
			Perfluorobutanoic acid	C_3F_7COOH	375-22-4
	S = Sulfonate or sulfonic acid	PFBS	Perfluorobutane sulfonate	$C_4F_9SO_3^-$	45187-15-3
			Perfluorobutane sulfonic acid	$C_4F_9SO_3H$	375-73-5
Pe = penta (5 carbon)	A = Carboxylate or carboxylic acid	PFPeA	Perfluoropentanoate	$C_4F_9CO_2^-$	45167-47-3
			Perfluoropentanoic acid	C_4F_9COOH	2706-90-3
	S = Sulfonate or sulfonic acid	PFPeS	Perfluoropentane sulfonate	$C_5F_{11}SO_3^-$	175905-36-9
			Perfluoropentane sulfonic acid	$C_5F_{11}SO_3H$	2706-91-4
Hx = hexa (6 carbon)	A = Carboxylate or carboxylic acid	PFHxA	Perfluorohexanoate	$C_5F_{11}CO_2^-$	92612-52-7
			Perfluorohexanoic acid	$C_5F_{11}COOH$	307-24-4
	S = Sulfonate or sulfonic acid	PFHxS	Perfluorohexane sulfonate	$C_6F_{13}SO_3^-$	108427-53-8
			Perfluorohexane sulfonic acid	$C_6F_{13}SO_3H$	355-46-4
Hp = hepta (7 carbon)	A = Carboxylate or carboxylic acid	PFHpA	Perfluoroheptanoate	$C_6F_{13}CO_2^-$	120885-29-2
			Perfluoroheptanoic acid	$C_6F_{13}COOH$	375-85-9
	S = Sulfonate or sulfonic acid	PFHpS	Perfluoroheptane sulfonate	$C_7F_{15}SO_3^-$	146689-46-5
			Perfluoroheptane sulfonic acid	$C_7F_{15}SO_3H$	375-92-8
O = octa (8 carbon)	A = Carboxylate or carboxylic acid	PFOA	Perfluorooctanoate	$C_7F_{15}CO_2^-$	45285-51-6
			Perfluorooctanoic acid	$C_7F_{15}COOH$	335-67-1
	S = Sulfonate or sulfonic acid	PFOS	Perfluorooctane sulfonate	$C_8F_{17}SO_3^-$	45298-90-6
			Perfluorooctane sulfonic acid	$C_8F_{17}SO_3H$	1763-23-1
N = nona (9 carbon)	A = Carboxylate or carboxylic acid	PFNA	Perfluorononanoate	$C_8F_{17}CO_2^-$	72007-68-2
			Perfluorononanoic acid	$C_8F_{17}COOH$	375-95-1
	S = Sulfonate or sulfonic acid	PFNS	Perfluorononane sulfonate	$C_9F_{19}SO_3^-$	474511-07-4
			Perfluorononane sulfonic acid	$C_9F_{19}SO_3H$	68259-12-1
D = deca (10 carbon)	A = Carboxylate or carboxylic acid	PFDA	Perfluorodecanoate	$C_9F_{19}CO_2^-$	73829-36-4
			Perfluorodecanoic acid	$C_9F_{19}COOH$	335-76-2
	S = Sulfonate or sulfonic acid	PFDS	Perfluorodecane sulfonate	$C_{10}F_{21}SO_3^-$	126105-34-8
			Perfluorodecane sulfonic acid	$C_{10}F_{21}SO_3H$	335-77-3

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

X	Y	Acronym	Name	Formula	CAS No.
Un = undeca (11 carbon)	A = Carboxylate or carboxylic acid	PFUnA or PFUnDA	Perfluoroundecanoate	$C_{10}F_{21}CO_2^-$	196859-54-8
			Perfluoroundecanoic acid	$C_{10}F_{21}COOH$	2058-94-8
	S = Sulfonate or sulfonic acid	PFUnS or PFUnDS	Perfluoroundecane sulfonate	$C_{11}F_{23}SO_3^-$	441296-91-9
			Perfluoroundecane sulfonic acid	$C_{11}F_{23}SO_3H$	749786-16-1
DoD = dodeca (12 carbon)	A = Carboxylate or carboxylic acid	PFDoDA	Perfluorododecanoate	$C_{11}F_{23}CO_2^-$	171978-95-3
			Perfluorododecanoic acid	$C_{11}F_{23}COOH$	307-55-1
	S = Sulfonate or sulfonic acid	PFDoDS	Perfluorododecane sulfonate	$C_{12}F_{25}SO_3^-$	343629-43-6
			Perfluorododecane sulfonic acid	$C_{12}F_{25}SO_3H$	79780-39-5
TrD = trideca (13 carbon)	A = Carboxylate or carboxylic acid	PFTrDA	Perfluorotridecanoate	$C_{12}F_{25}CO_2^-$	862374-87-6
			Perfluorotridecanoic acid	$C_{12}F_{25}COOH$	72629-94-8
	S = Sulfonate or sulfonic acid	PFTrDS	Perfluorotridecane sulfonate	$C_{13}F_{27}SO_3^-$	NA
			Perfluorotridecane sulfonic acid	$C_{13}F_{27}SO_3H$	NA
TeD = tetradeca (14 carbon)	A = Carboxylate or carboxylic acid	PFTeDA	Perfluorotetradecanoate	$C_{13}F_{27}CO_2^-$	365971-87-5
			Perfluorotetradecanoic acid	$C_{13}F_{27}COOH$	376-06-7
	S = Sulfonate or sulfonic acid	PFTeDS	Perfluorotetradecane sulfonate	$C_{14}F_{29}SO_3^-$	NA
			Perfluorotetradecane sulfonic acid	$C_{14}F_{29}SO_3H$	NA

NA = not available

Note that for carboxylates, the total number of carbons used for naming the compound includes the carbon in the carboxylic acid functional group (COOH), and so although PFOA has seven carbons in its fluoroalkyl tail, all eight of the carbons in the molecule are used to name it, hence *perfluorooctanoate*. However, in terms of chemical behavior, PFOA would be more analogous to seven-carbon perfluoroheptane sulfonate, PFHpS, than to eight-carbon perfluorooctane sulfonate, PFOS.

Note that in Table 3-1, PFAA names and formulas are shown in both the anionic (also referred to as “deprotonated”) and acid (or neutral; also referred to as protonated) forms. The anionic form is the state that PFAAs are found in the environment, except in very rare situations (for example, extremely low pH). The anionic and acid forms of PFAA names are often incorrectly used interchangeably (for example, perfluorooctane sulfonate and perfluorooctane sulfonic acid), and the same acronym (in this case, PFOS) applies to both forms. However, as discussed in Sections 3.2 and 6.2.2, their physical and chemical properties are different and it is important to know which form is being described.

Until recently, carboxylates and sulfonates have been the classes most commonly tested for in the environment. However, a wide range of PFAS with other functional groups exist for which the same “PFXY” shorthand shown above may or may not apply. For naming conventions for these compounds, please refer to Buck et al. (2011).

A Note About PFAS Naming in Laboratory Reports

Even though PFAAs occur as anions in the environment, some laboratories report all of their results in the acidic form, while others may report PFCAs as acids (for example, perfluorooctanoic acid) and PFSAAs as anions (for example, perfluorooctane sulfonate). Different naming conventions in laboratory reports has led to confusion regarding exactly which form of the PFAA they are measuring. Although the lab is measuring the concentration of PFAA anions present in the sample, where the results are reported as an acid, the lab has adjusted for the H⁺ cation (which has so little mass, this does not affect the resulting concentration).

It should be noted that the standards used by laboratories to perform analyses may be prepared from PFAA salts, as is often the case for sulfonate standards. If so, the lab must adjust the reported concentration to account for the mass of the counterion (typically Na⁺ or K⁺). The calculation to do this is described in Section 7.2.3 of EPA Method 537 (Shoemaker, Grimmatt, and Boutin 2009).

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

3.1 Long Chain versus Short Chain Distinction

PFAAs are sometimes described as *long-chain* and *short-chain* as a shorthand way to group PFCAs and PFSAAs that may behave similarly in the environment. However, it is important not to make generalizations about PFAA behavior based only on chain length. As recent research suggests, other factors besides chain length may affect bioaccumulation potential of PFAS (Ng and Hungerbühler 2014).

According to the Organisation for Economic Co-operation and Development (OECD 2013):

- *Long-chain* refers to:
 - o perfluoroalkyl carboxylic acids, PFCAs, with eight or more carbons (seven or more carbons are perfluorinated)
 - o perfluoroalkane sulfonates, PFSAs, with six or more carbons (six or more carbons are perfluorinated)
- *Short-chain* refers to:
 - o perfluoroalkyl carboxylic acids with seven or fewer carbons (six or fewer carbons are perfluorinated)
 - o perfluoroalkane sulfonates with five or fewer carbons (five or fewer carbons are perfluorinated)

Table 3-2 illustrates the differences in the short-chain and long-chain PFCAs and PFSAs.

Table 3-2. 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					

3.2 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 (see Section 6). 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 (see Table 3-1). 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:
 - o PFOS, acid form CAS No.: 1763-23-1
 - o PFOS, potassium salt CAS No.: 2795-39-3
 - o PFOS, ammonium salt CAS No.: 29081-56-9
- When the salt or acid exists in water or other liquids, it will dissociate and the salt or acid will break off and form the anion (COO⁻). Figure 3-1 illustrates the dissociation of perfluorobutanoic acid.
- It is most important to distinguish between the acid form and anionic form when reporting the physical and chemical properties. The discussion of PFAS properties in this fact sheet generally refers to the anionic form; it will be specifically called out if the acid form is being discussed.

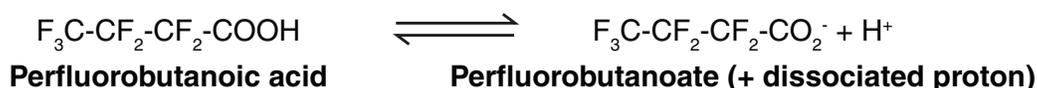


Figure 3-1. Dissociation of perfluorobutanoic acid

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

4 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 and may provide an indicator of their source. Structural differences are described below:

- A *linear isomer* is composed of carbon atoms bonded to only one or two carbons, which form a straight carbon backbone. There can be only one linear isomer in a C_n homologue (compounds with the same number of carbons in their tail) series.
- In a *branched isomer*, at least one carbon atom is bonded to more than two carbon atoms, which forms a branching of the carbon backbone. There can be many isomers per C_n homologue series.

Figure 4-1 illustrates the structures of linear and branched PFOS.



Figure 4-1. Linear and one branched isomer of PFOS

The formula “C_nF_{2n+1}” (where n is greater than or equal to 3) includes linear and branched structures. For example, PFOS and PFHxS are routinely present in environmental samples as a mixture of linear and branched isomers.

Accurate quantification of PFAS that are mixtures of linear isomers and branched isomers in environmental matrices can be difficult (Riddell et al. 2009). However, they 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 (see Table 4-1 and the *History and Use Fact Sheet*). The presence of linear and branched isomers may also have implications for partitioning and transport.

Table 4-1. Manufacturing processes and potential PFAAs produced

Manufacturing Process	Commonly Found Polyfluorinated Substance (Precursors)	Potential PFAAs Produced
Telomerization	FTSA ¹	Linear PFCAs
	FTCA ²	Linear PFCAs
	FTOH	Linear PFCAs
Electrochemical Fluorination	FASE	Branched and Linear PFCAs Branched and Linear PFSAs
	FASAA	Branched and Linear PFCAs Branched and Linear PFSAs
¹ Fluorotelomer sulfonate: found at AFFF sites ² Fluorotelomer carboxylic acids (for example, 5:3 Acid) found in landfill leachate		

5 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 chemistries that should not degrade to long-chain PFAAs (USEPA 2006a; OECD 2017). The short-chain alternatives include 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 et al. 2013; Buck 2015). While a full discussion of such 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.

Examples of this trend are replacement PFAS that have been developed for use as processing aids in the manufacturing of fluoropolymers. The replacements are generally fluorinated ether carboxylates. Two of these that have been detected

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

in the environment and generated public concern and regulatory actions are given here (their molecular structures are illustrated in Figure 5-1):

- GenX—trade name for ammonium, 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy) propanoate ($\text{CF}_3\text{CF}_2\text{CF}_2\text{OCF}(\text{CF}_3)\text{COO}^- \text{NH}_4^+$; CAS No. 62037-80-3), a perfluoropolyether carboxylate surfactant (Wang et al. 2013; Buck 2015)
- ADONA—trade name for ammonium 4,8-dioxa-3H-perfluorononanoate ($\text{CF}_3\text{OCF}_2\text{CF}_2\text{CF}_2\text{-OCHF}(\text{CF}_2)\text{COO}^- \text{NH}_4^+$ (CAS No. 958445-44-8), a polyfluoropolyether carboxylate surfactant (Gordon 2011)

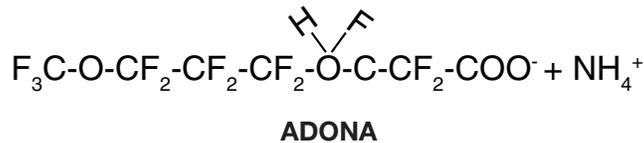
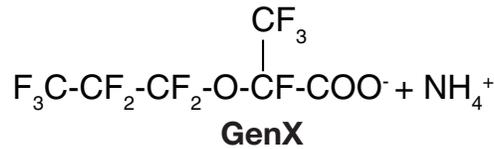


Figure 5-1. Example replacement chemistry structures

6 Physical and Chemical Properties

The physical and chemical properties of PFAS, in concert with the characteristics of the environmental system, determine the environmental behavior of organic contaminants, including the compound's state and partitioning behavior (Banks, Smart, and Tatlow 1994). Partitioning can occur between neutral and ionic molecular forms, solid and liquid states, and between different media and biota (aqueous, pure phase, soil/sediment, biota, and atmospheric). The environmental behavior of many PFAS is further complicated by their surfactant properties.

Figure 6-1 illustrates key chemical and physical properties and distribution coefficients. Comparing the chemical and physical properties of different PFAS provides insight into similarities and differences in their environmental behavior and can inform investigation design.

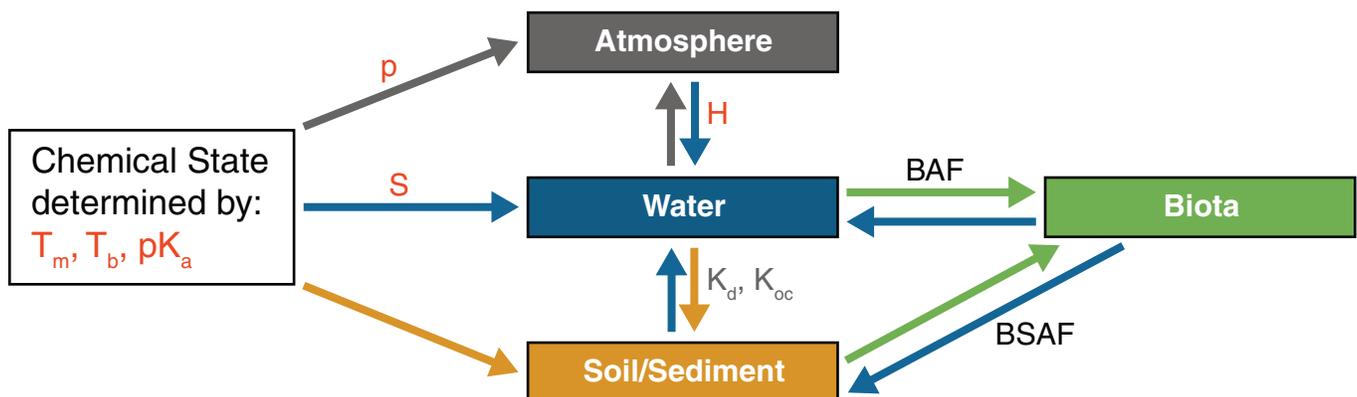


Figure 6-1. The role of key physical and chemical properties (shown in red) in influencing environmental compound behavior. Other key distribution coefficients (for example, K_d , K_{oc} shown in grey) are addressed in the *Environmental Fate and Transport Fact Sheet*. T_m = melting point; T_b = boiling point; pK_a = acid dissociation constant; p = vapor pressure; S = solubility; H = dimensionless Henry's law constant; K_d = soil and sediment partitioning coefficient; K_{oc} = organic carbon partitioning coefficient; BAF = bioaccumulation factor; and $BSAF$ = biota-sediment accumulation factor.

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

There is a large variation in published data on chemical and physical properties of PFAS. Reliable physical and chemical properties of PFAS are scarce (for example, vapor pressure and Henry's law constants), and some of the available values are modeled, as opposed to directly measured. With a few exceptions (Koc and BCF or BAF values), many of the available properties are based on the acid form of the PFAA, which is not present in the environment, unless at pH <3, which is not typical. Table 6-1 provides a general summary of the available chemical and physical property information for PFCAs and the sensitivity of this information in relation to the acid vs. anionic form. For example, the anionic forms of PFOA and PFOS have documented bioconcentration factor and bioaccumulation factor properties (Martin et al. 2003a; 2003b) while other properties are not readily available.

Table 6-1. Available physical and chemical properties for PFCAs

Properties								Environmentally Relevant?
PFAA State	CAS No.	S _w	P ^o	K _h	K _{ow}	K _{oc}	BCF and/or BAF	
Acid	Y	Y	Y	E	E	E	N	No
Cation:								No
NH ₄ ⁺	Y	Y	N	N	N	N	N	
Li ⁺	Y	Y	N	N	N	N	N	
Na ⁺	Y	Y	N	N	N	N	N	
Anion	M	N	N	N	N	Y	Y	Yes

S_w = solubility in water

P^o = vapor pressure

K_h = Henry's Law Constant

K_{ow} = octanol/water partition coefficient

K_{oc} = organic carbon partition coefficient

BAF = bioaccumulation factor

BCF = bioconcentration factor

Y = data available

N = no data available

M = data may be available for some

E = data estimated, not directly measured

6.1 Physical Properties

Many PFAS are in solid form at room temperature, often as a white powder or waxy substance, though some may be liquids. As mentioned before, data regarding physical properties of PFAS are scarce, and for PFAAs may relate to the acid form of the compound, which is not the most environmentally relevant form. Some melting point data are available for standards of PFCAs in the acid form. Measured vapor pressures for the acid form of PFOA, PFNA, PFDA, PFUnA, and PFDoA (Barton, Botelho, and Kaiser 2008; Kaiser et al. 2005) and fluorotelomer alcohols (Krusic et al. 2005) are also available. Similarly, Henry's Law constants are available for fluorotelomer alcohols (Goss et al. 2006). For PFAAs, the acid form is known to partition into air from aqueous solutions at very low pH (Kaiser et al. 2010). Care should be taken when reviewing available physical property information for PFAS to ensure that it applies to the form (for example, acid or anionic) of concern to the project or site in question.

6.2 Chemical Properties

6.2.1 Fluorine and the Carbon-fluorine (C-F) Bond

As previously mentioned, understanding PFAS chemical properties is key to understanding the diversity of uses and applications associated with this class of compounds, as well as their unique environmental behavior. Some key fluorine chemical properties and the characteristics they impart to PFAS are provided in Table 6-2.

Properties such as the high electronegativity and small size of fluorine lead to a strong C-F bond, the strongest covalent bond in organic chemistry (Kissa 2001; Banks, Smart, and Tatlow 1994). The low polarizability of fluorine further leads to weak intermolecular interactions, such as van der Waals interactions and hydrogen bonding (Kissa 2001; Banks, Smart, and Tatlow 1994). It is mainly the unique properties of fluorine that give many PFAS their mutually hydro- and lipophobic (stain-resistant) and surfactant properties and make them thermally and chemically stable. Not all of these characteristics (for example, surface activity) are universal to all PFAS.

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

Table 6-2. Fluorine characteristics, resulting characteristics and properties of PFAS

Fluorine Characteristic	Description	Result	Resulting Property of PFAS
High electronegativity	Tendency to attract shared electrons in a bond	Strong C-F bond	Thermal stability
			Chemical stability (low reactivity)
		Polar bond with partial negative charge towards F	Strong acidity (low pKa) ¹
Low polarizability	Electron cloud density not easily impacted by the electric fields of other molecules	Weak intermolecular interactions (for example, van der Waals, hydrogen bonds)	Hydrophobic and lipophobic surfactant properties ²
		Low surface energy	
Small size	Atomic radius of covalently bonded fluorine is 0.72 Å	Shields carbon	Chemical stability (low reactivity)

¹When paired with an acid functional group such as a carboxylic or sulfonic acid
²When paired with a functional group that is hydrophilic (for example, a carboxylate)
 Å = Angstrom

6.2.2 Acid Dissociation Constants

Knowing whether a chemical will dissociate in other liquids is important to understanding its fate and transport in the environment. The acid dissociation constant (K_a) is a quantitative measurement of the strength of an acid in solution, although it is usually presented in the form of the logarithmic constant (pK_a). The larger the value for pK_a , the smaller the extent to which the chemical will dissociate at a given pH. Chemicals with small pK_a values are called *strong acids* and those with large pK_a values are called *weak acids*.

Many PFAAs, such as PFCAs and PFSAAs, are strong acids due to the electron withdrawing effects of fluorine extending to their acid functional groups (Kissa 2001, Banks, Smart, and Tatlow 1994). As a result, most PFAAs readily dissociate in water and other environmental matrices. Therefore, at most environmentally relevant pHs, PFCAs and PFSAAs are present in the dissociated anionic form rather than the acid form.

The acid and anionic forms have very different physical and chemical properties. For example, perfluorooctanoate anion is highly water soluble and has negligible vapor pressure, whereas perfluorooctanoic acid has very low water solubility and sufficient vapor pressure to partition out of water into air. It is essential to distinguish between the acid form and the anionic form when looking at physical and chemical properties or fate and transport evaluations.

Specific pK_a values for PFAAs are generally not available. Limited model-predicted and experimental values are available for PFOA, and range from -0.5 to 3.8 (Burns et al. 2008; Kissa 2001; Barton, Kaiser, and Russell 2007; Goss 2008), suggesting that at nearly neutral pH (near $pH = 7.0$), PFOA will exist in the aqueous phase in anionic form and the amount of acid PFOA in most environmentally relevant systems will be negligible. A recent study estimates that the pK_a values of PFBA, PFHxA, PFHpA, PFOA, PFNA, PFDA, and PFUnA are all less than 1.6 and pK_a values of PFSAAs are expected to be even lower (Vierke, Berger, and Cousins 2013).

6.2.3 Thermal and Chemical Stability

Terminal PFAAs, such as PFOA and PFOS, are extremely stable, thermally and chemically, and resist degradation and oxidation. Thermal stability of PFAAs is primarily attributable to the strength of the C-F bond in the fluoroalkyl tail (Kissa 2001). The stability is determined by the specific functional group that is attached to the fluoroalkyl tail. PFCAs and PFSAAs are the most stable fluorinated surfactants. The acid forms of these PFAAs decompose at temperatures greater than 400°C, but complete mineralization occurs at temperatures greater than 1000°C. In a practical situation like a municipal incinerator, the mineralization temperature may be lower due to the presence of other substances that contain hydrogen. The thermal stability is lower for the salts of PFAA compounds and depends on which cation is the counter ion. For example, the 20% decomposition temperature of sodium perfluorooctanoate is 298°C, but is 341°C for lithium perfluorooctanoate (Kissa 2001). Additionally, salts of PFSAAs are more thermally stable than the corresponding salts of PFCAs (Kissa 2001).

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

The strength of the C-F bond, shielding of carbon by fluorine, and inductive effects (caused by fluorine electronegativity) also lead to PFAS chemical stability. For example, electron-rich chemical species called nucleophiles normally would be attracted to the partial positive charge of carbon. If they can get close enough to the carbon to bond with it, this would eliminate a fluorine from the molecule, making it vulnerable to degradation. However, the size of the fluorine atoms surrounding the carbon prevents this from happening (Banks, Smart, and Tatlow 1994; Schwarzenbach, Gschwend, and Imboden 2003). This is why processes such as hydrolysis, which involve eliminating one or more fluorines, are ineffective at degrading PFAAs. Similarly, many PFAAs are resistant to degradation by oxidative processes that rely on a loss of electrons (Kissa 2001). PFAAs are also resistant to reductive processes, which involve gaining electrons. Despite having a high affinity for electrons, fluorine does not have vacant orbitals favorable for accepting additional electrons (Park et al. 2009).

6.2.4 Octanol/Water Partition Coefficient, K_{ow}

The octanol/water partition (K_{ow}) coefficient is sometimes used as a proxy for uptake in biological systems. The K_{ow} value is defined as “the ratio of a chemical’s concentration in the octanol phase to its concentration in the aqueous phase of a two-phase [octanol/water system]” (USEPA 2015d). The vapor pressure, melting point, and boiling point of neutral, volatile, nonpolymeric PFAS (for example, FTOH) can be measured, and K_{ow} can be either estimated or measured. The K_{ow} values that are typically tabulated for the PFCAs and PFSAAs are for the acid form and are therefore not relevant because PFCAs and PFSAAs are anionic at environmental pHs. Additionally, because many PFAS bind to proteins (proteinphiles), some PFAS may bioaccumulate by mechanisms other than those that drive more traditional hydrophobic contaminants (Ng and Hungerbühler 2013; 2014). Other PFAS may simply be detected in organisms due to ongoing exposures and their extended human half-lives (for example, concentrations in drinking water) (Wiesmueller 2012; Gyllenhammar et al. 2015). It should be noted that although the K_{ow} for some organic contaminants can be used for estimating K_{oc} , this cannot be performed for estimating values for PFAS.

7 Summary

This fact sheet addresses naming conventions and physical and chemical properties 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). In general, values for physical and chemical properties of many nonpolymeric PFAS are not available. With the 2015 major global manufacturer phase-out of long-chain PFAAs and their potential precursors, such as those based on C8 chemistry (see *History and Use Fact Sheet*), replacement PFAS (for example, short-chain alternatives and nonpolymer perfluoropolyethers) have been commercially introduced (many following review by USEPA) and may continue to be developed. In the future, it may be necessary to expand the current naming conventions and acronym approaches to ensure that standardized naming is available for additional members of the PFAS class of compounds. Further, additional information on physical and chemical properties of these compounds may become available as increased numbers of PFAS are included in environmental and human health-related studies. Refer to the other PFAS fact sheets for further information on these properties and how they are practically applied.

8 References and Acronyms

The references cited in this fact sheet, and the other ITRC PFAS fact sheets, are included in one combined list that is available on the ITRC web site. The combined acronyms list is also available on the ITRC web site.



Per- and Polyfluoroalkyl Substances (PFAS) Team Contacts

Robert Mueller • New Jersey Department of Environmental Protection
609-984-3910 • Bob.Mueller@dep.nj.gov

Virginia Yingling • Minnesota Department of Health
651-343-2890 • virginia.yingling@state.mn.us

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ITRC
1250 H St. NW, Suite 850
Washington, DC 20005
itrcweb.org



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