

# Report back on [Buck et al. \(2011\)](#) definition of perfluoroalkyl and polyfluoroalkyl substances (PFASs)

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Office of Environmental Health Hazard Assessment (OEHHA)  
Biomonitoring California Scientific Guidance Panel (SGP) Meeting  
March 25, 2022

Buck et al. (2011), Integr Environ Assess Manag 7(4):513–541

# Background

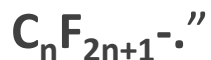
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- Biomonitoring California relies on the Buck et al. (2011) definition for the class of perfluoroalkyl and polyfluoroalkyl substances (PFASs).
- PFASs as a class were recommended by the SGP for addition to Biomonitoring California's lists of:
  - [Designated chemicals](#) in March 2015. These are the entire pool from which the Program can select chemicals to biomonitor.
  - [Priority chemicals](#) in November 2015. These are the SGP's priorities to biomonitor in California.
- At the November 2021 SGP meeting, OEHHA was asked to report back on the Buck et al. definition in terms of PFASs that may be missed.

# Excerpt 1 from Buck et al. (p. 515)

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“As defined above, PFASs are **aliphatic** substances containing one or more C atoms on which all the H substituents present in the nonfluorinated analogues from which they are notionally derived have been replaced by F atoms, in such a manner that PFASs contain the **perfluoroalkyl moiety**



**Emphasis added**

# Excerpt 2 from Buck et al. (p. 515)

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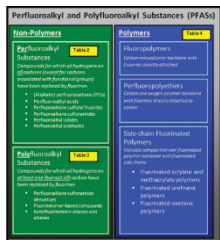
“More explicitly, we recommend that the family of compounds denoted by the acronym PFAS should encompass:

- **Perfluoroalkyl** substances, which are defined as aliphatic substances for which **all of the H atoms attached to C atoms** in the nonfluorinated substance from which they are notionally derived **have been replaced by F atoms**, except those H atoms whose substitution would modify the nature of any functional groups present...”

# Excerpt 2 (cont.) from Buck et al. (p. 515)

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- **“Polyfluoroalkyl** substances, defined here as aliphatic substances for which all H atoms attached to **at least one (but not all) C atoms have been replaced by F atoms**, in such a manner that they **contain the perfluoroalkyl moiety  $C_nF_{2n+1}-$  (e.g.,  $C_8F_{17}CH_2CH_2OH$ )**. Thus, whereas the general chemical concept of “polyfluorination” embraces compounds containing “scattered” multiple F atoms (such as in  $CH_2FCHFCHFCH_2OH$ ), as well as “grouped” ones (such as in  $CF_3CF_2CH_2COOH$ ), we consider that only those polyfluorinated substances having at least one perfluoroalkyl moiety  $C_nF_{2n+1}-$  belong to the PFAS family.”



Adapted from Buck et al. (p. 521)

Figure 4. Classification hierarchy of environmentally relevant perfluoroalkyl and polyfluoroalkyl substances (PFASs)

# Perfluoroalkyl and Polyfluoroalkyl Substances (PFASs)

## Non-polymers

### Perfluoroalkyl Substances

Table 2

*Compounds for which all hydrogens on all carbons (except for carbons associated with functional groups) have been replaced by fluorines*

- (Aliphatic) perfluorocarbons (PFCs)
- Perfluoroalkyl acids
- Perfluoroalkane sulfonyl fluorides
- Perfluoroalkane sulfonamides
- Perfluoroalkyl iodides
- Perfluoroalkyl aldehydes

### Polyfluoroalkyl substances

Table 3

*Compounds for which all hydrogens on at least one (but not all) carbon have been replaced by fluorines*

- Perfluoroalkane sulfonamido derivatives
- Fluorotelomer-based compounds
- Semifluorinated *n*-alkanes and alkenes

## Polymers

Table 4

### Fluoropolymers

*Carbon-only polymer backbone with fluorines directly attached*

### Perfluoropolyethers

*Carbon and oxygen polymer backbone with fluorines directly attached to carbon*

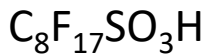
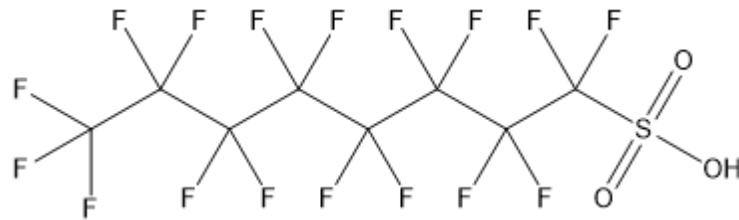
### Side-chain Fluorinated Polymers

*Variable composition non-fluorinated polymer backbone with fluorinated side chains*

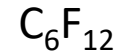
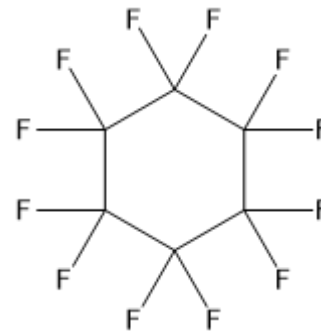
- Fluorinated acrylate and methacrylate polymers
- Fluorinated urethane polymers
- Fluorinated oxetane polymers

# Example chemicals to illustrate interpretation of Buck et al.

Perfluorooctanesulfonic acid (PFOS)



Perfluorocyclohexane



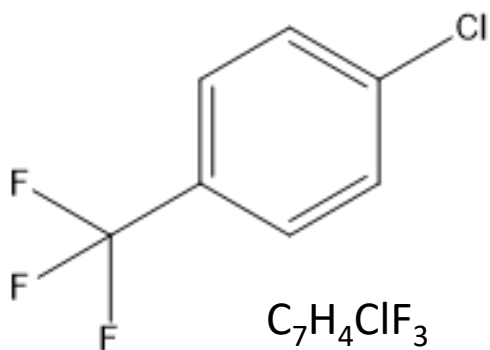
Moiety is  $C_nF_{2n+1}^-$

Selected fluoropolymers

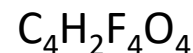
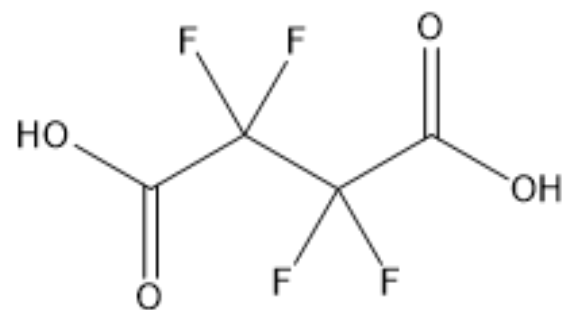
Polytetrafluoroethylene	PTFE	$-(CF_2CF_2)_n-$
Polyvinylidene fluoride	PVDF	$-(CH_2CF_2)_n-$
Polyvinyl fluoride	PVF	$-(CH_2CHF)_n-$

# Examples chemicals (cont.)

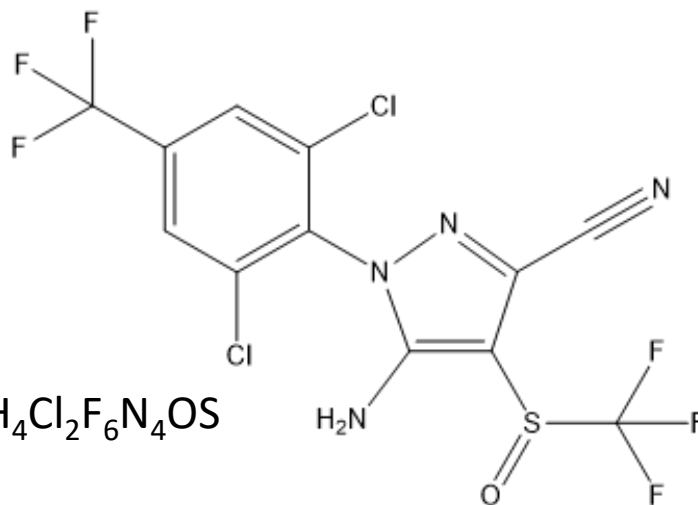
*para*-Chlorobenzotrifluoride



Tetrafluorosuccinic acid



Fipronil



Moiety is  $C_nF_{2n+1}^-$



# Interim step - clarify current PFAS footnote

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- Current language:

PFASs are fluorinated aliphatic substances that contain the moiety  $C_nF_{2n+1}^-$ . In a perfluoroalkyl substance, all carbon atoms, except for carbon atoms associated with functional groups (such as an aldehyde group), are fully fluorinated. In a polyfluoroalkyl substance, at least one (but not all) of the carbon atoms is fully fluorinated. For complete technical details on the definition of PFASs, see Buck et al. (2011).

- Proposed simplification:

Refer to Buck et al. (2011) for the description of PFASs and example members of this class.

# Proposed future steps

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- Evaluate definitions of PFASs from other groups, such as:
  - [OECD 2021](#) (summarized in [Wang et al., 2021](#))
  - [Glüge et al., 2020](#)
- Consider adapting language used in some PFAS bills (e.g., California [SB 1044](#))
  - Fluorinated organic chemicals containing at least one fully fluorinated carbon atom.
- Develop a definition designed to address Program needs/priorities. For example:
  - Retain reference to Buck et al. to keep all currently listed PFASs, including specified polymers
  - Add a phrase to expand the definition to include relevant fluorinated chemicals not already clearly captured by Buck et al.
  - Could consider functional descriptor(s)

# Feedback requested today

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- Comments on simplification of current PFAS footnote
- Input on proposed future steps, including:
  - Suggestions on which alternative PFAS definitions to evaluate
  - Possible approaches for developing a definition to meet Program needs and priorities

Send comments at any time to  
[biomonitoring@oehha.ca.gov](mailto:biomonitoring@oehha.ca.gov)