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Viewpoint

A New OECD Definition for Per- and Polyfluoroalkyl Substances

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Per- and polyfluoroalkyl substances (PFASs) comprise a class of chemicals that has attracted much attention since the early 2000s, when the hazards and ubiquitous occurrence of two PFASs—perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS)—were reported. Early communications used multiple terms such as "per- and polyfluorinated chemicals", "perfluorinated organics", "perfluorochemical surfactants", and "highly fluorinated compounds". In 2011, to harmonize communication, Buck et al.[1] published a milestone paper, providing the first clear structural definition of PFASs and recommendations on the names and acronyms for over 200 individual PFASs. Since then, research and regulation has expanded from PFOA and PFOS to a much wider range of substances.

In 2018, the so-called "Global PFC Group" led by the Organisation for Economic Co-operation and Development (OECD) and the United Nations Environment Programme (UNEP) published a list of over 4700 PFASs that contain a $-C_nF_{2n}-$ ($n \geq 3$) or $-C_nF_{2n}OC_mF_{2m}-$ (n and $m \geq 1$) moiety and that were known or likely to have been on the global market.[2] The list included substances that contain fully fluorinated carbon moieties, but do not meet the PFAS definition in Buck et al. (2011) due to a lack of a $-CF_3$ group in the molecule. Additionally, recent advancement of nontargeted analytical techniques enabled identification of many unknown PFASs in environmental and product samples. These developments provided motivation to reconcile the terminology of the PFAS universe, including a renewed look at the PFAS definition.

Against this backdrop, a report on the terminology of PFASs was recently published under the framework of the Global PFC Group.[3] This report reflects a three-year multistakeholder

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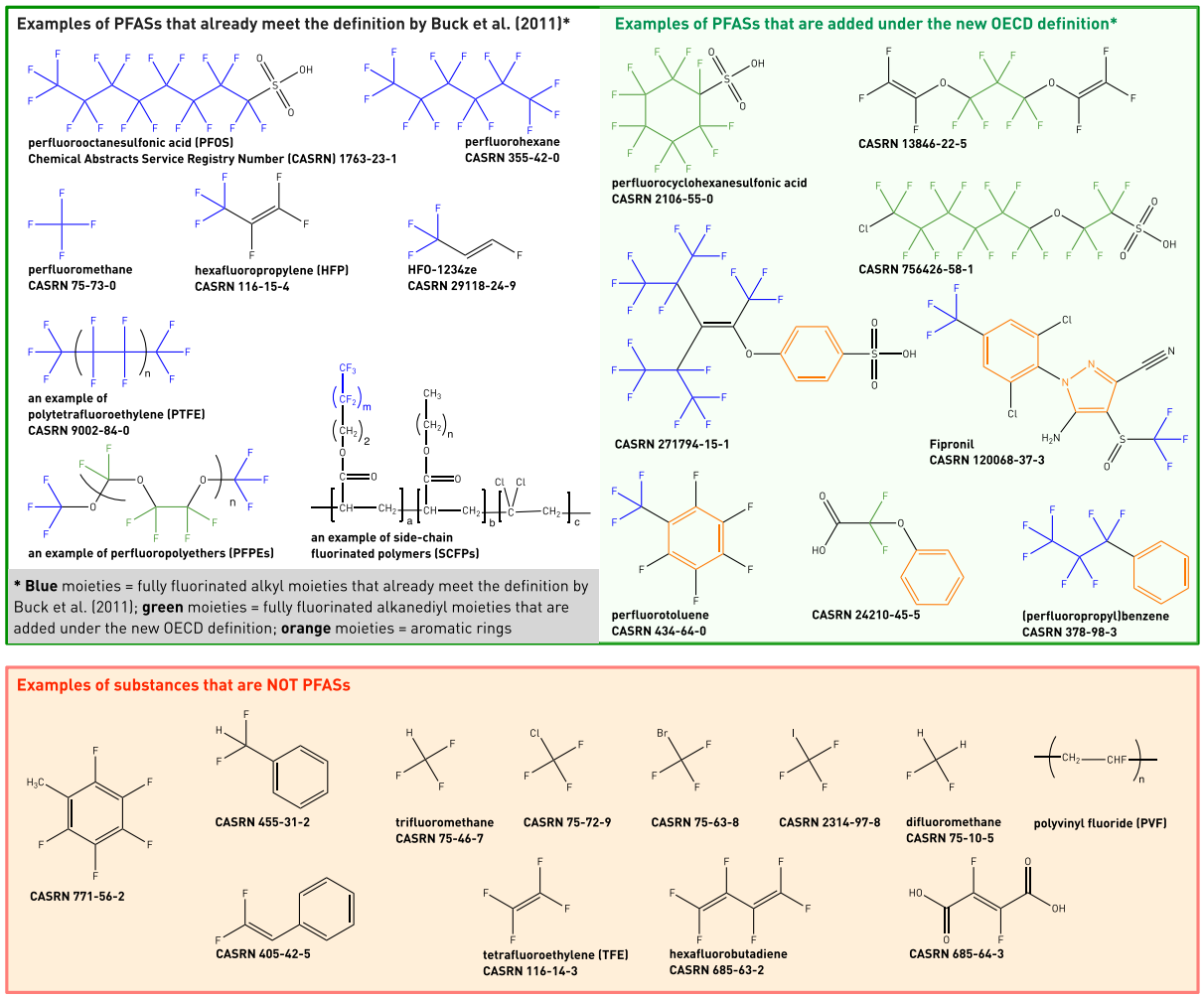

Figure 1. Examples of substances that are, and are not, PFASs based on the new definition.

international effort in reviewing the universe and terminology of PFASs to provide recommendations and practical guidance. We encourage stakeholders from academia, civil society, industry, and government to read the report and consider adopting its recommendations, wherever feasible, to help enable the coherent and consistent use of PFAS terminology across sectors and around the world. This Viewpoint provides an overview of the report.

A REVISED PFAS DEFINITION

The report details four major limitations with the previous definition in representing the PFAS universe: (1) omission of substances that have functional groups on both ends of the fully fluorinated carbon moiety (e.g., perfluoroalkyldicarboxylic acids); (2) inconsistencies in dealing with homologues that are fully fluorinated aliphatic cyclic compounds with or without a fully fluorinated alkyl side chain; (3) omission of substances with aromatic ring(s) in the nonfluorinated functional group(s) that can be cleaved in the environment and biota; and (4) use of the ambiguous term "highly fluorinated".

To address these concerns, the report presents a revised, broadly inclusive PFAS definition: "*PFASs are defined as fluorinated substances that contain at least one* **fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)**, *i.e., with a few noted exceptions, any chemical with at least a perfluorinated methyl group ($-CF_3$) or a perfluorinated methylene group ($-CF_2-$) is a PFAS*". The "noted exceptions" refer to a carbon atom with a H/Cl/Br/I atom attached to it.

The rationale behind the revision is to have a coherent and consistent definition across compounds from the view of the chemical structure. The new definition was required to be easily implementable for distinguishing between PFASs and non-PFASs, and easily understood by experts and nonexperts alike. Figure 1 illustrates examples that are, and are not, PFASs. This revised definition captures the broadness of the PFAS universe, ranging from small molecules, to more complex aromatics with a perfluorinated methyl/methylene group on the side chain(s), to diverse polymers.

Building on the revised definition, the report further provides (1) an explanation of how PFASs relate to other organofluorine compounds, (2) a comprehensive overview of known PFAS groups and their structural traits, including examples and notes on whether common names and acronyms

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exist, and (3) some common synthesis routes of individual or groups of PFASs.

PRACTICAL GUIDANCE ON HOW TO USE THE PFAS TERMINOLOGY

The report highlights the need to distinguish between the general definition and user-specific working scopes of PFASs. The general definition is based on molecular structure alone and serves as a starting and reference point to guide individual users to have a comprehensive understanding of the scale and diversity of chemicals in the PFAS universe. Meanwhile, users may define their own working scope of PFASs for specific activities according to their specific needs by combining the general definition with additional considerations (e.g., specific properties, use areas). When such a working scope of PFASs is used, the report recommends that respective users clearly provide the context and rationale for selecting their working scope to ensure transparency and avoid confusion by others.

The report further recommends using and building upon existing common terminologies such as in Buck et al. (2011) and well-defined common practices in organic chemistry, unless it is essential to deviate from them, to keep the consistent and coherent use of the PFAS terminology. As PFASs are a chemical class with diverse molecular structures and thus properties, it is recommended to properly recognize and communicate such diversity in a clear, specific and descriptive manner.

A SYSTEMATIC MOLECULAR STRUCTURE-BASED APPROACH TO CHARACTERIZING PFASS

When users define their own working scope of PFASs, they need to determine whether a compound falls or does not fall into their working scope. However, given the complexity and diversity of PFASs, it can be a challenging task to characterize and categorize PFASs based on chemical structures in a coherent and consistent manner, particularly for nonexperts. Different users may have different construction of working scopes, and there is no single categorization/grouping system that suits all. Therefore, the report provides a standardized approach for systematically characterizing PFASs based on molecular structural traits that will allow stakeholders to make their own categorization in a coherent and consistent manner. This system can be used to manually characterize and categorize PFASs, but the approach could also be used as inputs for developing automated cheminformatic tools.[4]

FUTURE WORK ON PFAS TERMINOLOGY

Four areas are recognized for further work to facilitate clear and unambiguous communication: (1) a centralized PFAS nomenclature database/platform; (2) development of cheminformatic tools for automated, structure-based systematic characterizaing and categorizing of PFASs; (3) work on the characterization and reporting of polymers; and (4) work on organofluorine compounds not currently defined as PFASs, including many fluorinated aromatics.

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Notes

The authors declare no competing financial interest.

Biography

Dr. Zhanyun Wang is a senior researcher in the Ecological Systems Design Group at ETH Zürich, Switzerland. As an environmental chemist by training, his research interests focus primarily on understanding the life cycles and risks of various anthropogenic chemicals in the technosphere and natural environment. He is also very interested in exploring novel and pragmatic approaches to advancing sound chemicals management, enabling a sustainable

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circular economy, and strengthening science-policy interface on chemicals and waste.

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