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Correspondence/Rebuttal

Comment on "Scientists' Statement on the Chemical Definition of PFASs"

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Sigmund et al.[1] raise unfounded concerns about an International Union of Pure and Applied Chemistry (IUPAC) project focused on the scientific definition of PFAS. These concerns reflect incorrect assumptions and a fundamental misunderstanding of how IUPAC projects are conducted. We outline the process by which IUPAC projects are typically carried out and discuss how the concerns by Sigmund et al.[1] are totally unjustified. To remove any doubt, we state that IUPAC is not a regulatory institution, and its task groups do not make any regulatory recommendations.

IUPAC is a global, not-for-profit, scientific organization with over 100 years of history. It brings together more than 50 national chemistry organizations and societies to establish international consensus on scientific issues related to all areas of chemistry. IUPAC has helped create the common language of chemistry by developing standardized chemical nomenclature, terminology, and data representation.

IUPAC achieves its goals through the collective efforts of global networks of experts who volunteer to design and conduct scientific, internally funded projects, resulting in published reports. Chemists from anywhere in the world can submit project proposals, which are carefully peer reviewed by IUPAC volunteers and external experts. The assigned international task groups (TGs) carry out the technical work that typically takes between one and five years. Projects usually yield technical reports or recommendations. Some projects also generate educational materials.

The process is guided by the IUPAC's Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS). Once a draft recommendation has been approved, it is released publicly as a provisional recommendation and open for public comment for four months. After final revisions, the recommendations are officially published in the IUPAC journal *Pure and Applied Chemistry* or one of IUPAC's reference books.[2] This lengthy and meticulous procedure, honed over more than a century, has proven to be an effective mechanism for establishing international standards for chemical terminology and nomenclature.

Per- and polyfluoroalkyl substances (PFAS) are a class of chemicals that have been used since the 1950s in a wide range of industrial and consumer applications. Some PFAS, such as PFOA (perfluorooctanoic acid, $C_7F_{15}C(O)OH$) and PFOS (perfluorooctanesulfonic acid, $C_8F_{17}S(O)_2OH$), are toxic, bioaccumulative, mobile, and persistent organic pollutants and are regulated under the Stockholm Convention.[3] Recognition of the hazardous nature of some PFAS and their widespread distribution and persistency within the environment has led to research, regulatory, and public interest in this class of compounds.

It is useful to recognize two general types of chemical definitions: scientific and regulatory. Scientific definitions for PFAS have evolved over time. Buck et al.[4] defined PFAS as "highly fluorinated aliphatic substances that contain one or more carbon atoms on which all the H substituents (present in the nonfluorinated analogs from which they are notionally derived) have been replaced by F atoms, in such a manner that they contain the perfluoroalkyl moiety $C_nF_{2n+1}-$". In 2018, the OECD defined[5] PFAS as "substances containing at least one $-C_nF_{2n}-$ ($n \geq 3$) or $-C_nF_{2n}OC_mF_{2m}-$ ($n, m \geq 1$) group". In 2021, the OECD expanded their definition to "substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)".[6] These exceptions and others make the OECD definition misaligned with an approach purely based on molecular structure and nomenclature.

IUPAC is well positioned, and its procedures are well suited to examine existing terminologies and classifications. On June 26, 2024, the Union initiated the project "Terminology and Classification of Per- and Poly-Fluoroalkyl Substances (PFAS)" (https://iupac.org/project/2024-006-3-100). The TG is collecting and critically analyzing existing information, classification, and nomenclature. The TG intends to propose recommendations for scientific terminology that are objective and consistent with existing IUPAC terminology, based on chemical structure.[7]

We assume that everyone involved in the terminology and classification of PFAS seeks to protect environmental and human health. No one can claim a monopoly on these assertions. While recognizing the potential influence of commercial interests, one should also be aware of the interests of politicians, environmental activists, and journalists, among others.

The IUPAC project has just commenced. Its findings are unknown and unpredictable, and it may take several years to reach provisional conclusions. Three aspects of the TG's work address the concerns raised by Sigmund et al.[1] First, the TG is

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large, comprising scientists and experts with diverse, heterogeneous backgrounds in chemistry. Second, the TG is open minded, considering all possibilities and inviting external advice and input from other individuals and organizations worldwide. Third, the TG's work will undergo multiple levels of peer review as described above.

IUPAC and the TG acknowledge the effort that led to the 2021 OECD definition of PFAS.[8] Therefore, there is no need to advertise and promote it as "*scientifically grounded, unambiguous, inclusive, well suited to identify these chemicals, should be the general basis for harmonized regulation*".[1] The lack of openness to improvement in the PFAS definition articulated by Sigmund et al.[1] is shortsighted. The TG has not finalized any conclusion; there are no indications that certain subgroups of chemicals would be excluded. Contrary to the concerns by Sigmund et al.,[1] it is possible that subgroups of chemicals *excluded* in the OECD definition would be *included* in a future IUPAC definition.

The above arguments address the scientific aspect of the article by Sigmund et al.[1] The other aspect concerns the code of conduct of science publishing. The ACS has instituted its Author Guidelines to filter out inappropriate practices and language that have unfortunately plagued social media and populist journalism. These Guidelines state that Highlight articles "*should express urgent information based on scientific research in an environmental discipline, that should not be political, personal, or summary in nature.*" However, interviews with the authors were disseminated through public media on the day their Highlight article was published, leading to inflammatory allegations and suggesting ulterior motives by IUPAC's volunteers. While scientific debate is a legitimate and constructive mechanism for advancing science, inappropriate *ad hominem* rhetoric has no place in scientific discourse.

We are disappointed in the ambiguity of the language used by Sigmund et al. in suggesting a hidden agenda, specifically the text that states: "*We are concerned that some individuals and organizations are seeking a redefinition of PFASs endorsed by the International Union of Pure and Applied Chemistry (IUPAC) to exclude certain fluorinated chemical subgroups from the scope of the existing definition. We are concerned that this effort is politically and/or economically, rather than scientifically, motivated.*" The Highlight by Sigmund et al. goes further "*Introducing an alternative or competing PFAS definition for general PFAS identification that includes considerations beyond chemical structure is concerning. It may be used by some parties with vested interests to influence regulations and, hence, which PFASs are allowed to be used, emitted, and occur in products and environments.*" We are not aware of any undue influence from individuals and organizations. As described above, the three mechanistic principles by which IUPAC TGs operate means views, opinions, contributions, and ideas are encouraged and welcomed from all stakeholders in a transparent process that is subject to external peer review and public scrutiny.

In conclusion, PFAS pose challenges that are too serious to be met by premature and hasty regulatory maneuvers. Organofluorine chemistry is a vibrant and rapidly evolving field that continually surprises the scientific community with numerous unexpected discoveries.[9,10] Following the common practice of all IUPAC projects, the Task Group is open to constructive criticism and collaboration, inviting input from a diverse range of stakeholders. We would greatly welcome and appreciate valuable input from Sigmund et al.[1] and other experts.

Timothy J. Wallington orcid.org/0000-0002-9810-6326
Pierangelo Metrangolo orcid.org/0000-0002-7945-099X
Bruno Ameduri orcid.org/0000-0003-4217-6664
Lidia Armelao
Valentina Dichiarante orcid.org/0000-0002-2977-5833
Hisao Hori orcid.org/0000-0003-3177-5282
Melanie Kah orcid.org/0000-0002-8705-9229
Rai Kookana orcid.org/0000-0002-0477-3284
Marie Pierre Krafft orcid.org/0000-0002-3379-2783
Sebastian Riedel orcid.org/0000-0003-4552-5719
Justyna Walkowiak-Kulikowska
Ehud Keinan orcid.org/0000-0002-7846-1080

AUTHOR INFORMATION

Complete contact information is available at:
https://pubs.acs.org/10.1021/acs.estlett.5c00642

Author Contributions

All authors contributed to conceptualization, writing, reviewing, and editing.

Notes

P.M. is currently engaged in contract research involving sensing, remediation, and destruction of PFAS. S.R. is currently engaged in contract research for SF_6 replacement substances and served as a paid expert witness. M.P.K is currently conducting contract research on the biodegradation and toxicity of PFAS. Views expressed here are those of the authors and not necessarily the views of the ACS.
The authors declare no competing financial interest.

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