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Recommended terms and abbreviations for polychlorinated alkanes (PCAs) as the predominant component of chlorinated paraffins (CPs)

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ABSTRACT

Despite several decades of study, ambiguities persist in terms used to express environmental and biotic occurrences of polychlorinated alkanes (PCAs), the main ingredient of chlorinated paraffins (CPs). This can lead to misinterpretation of data between analytical chemists, toxicologists, risk assessors/managers and regulators. The terms recommended here to harmonise reporting and reduce ambiguity use the conventional definition of PCAs - linear chlorinated alkanes (typically, $C_{\geq 10}$) with one chlorine per carbon, although some evidence of multiple chlorination exists. Other recommendations include.

- reporting the "Sum of measured PCAs" because "Total PCAs" is currently unquantifiable.
- reporting individual chain lengths, e.g., ΣPCAs-C_{11}, ΣPCAs-C_{13}, allows easier comparability and allows toxicology and risk assessment to consider different PCA combinations.
- maintain studies on individual PCAs in order to better characterise chemical, environmental and health risk behaviour.

The terms could be extended in future to assimilate new findings on individual PCAs, multiple chlorination and chirality.

1. Introduction

Chlorinated paraffins (CPs) are industrial chemicals that have been manufactured and used for almost a century and are still produced in huge volumes. Although there was significant use of CPs during the first world war, the commercial application of the product as a pressure additive in lubricating oils saw the first large scale production in the US starting in 1932 [1]. Historically, the largest production volumes were seen in Europe and North America but these were surpassed by China during the mid-1990s [2]. Current global production is estimated

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between 1.5 and 2 million tonnes per year [2,3] of which China and India account for the largest amounts.

The diverse applications of CPs have witnessed temporal changes which also vary by region. Early wide-scale use for weather- and flame-proofing of military materials in the US during and after the Second World War gave way to the most common application as a machining fluid which still accounts for a significant proportion of global usage. However, the use of CPs as a secondary plasticizer and flame retardant in polyvinylchloride (PVC) manufacture is the largest current application, particularly in Europe and China [2,4]. In addition to CPs, smaller quantities (<1000 tonnes/year during peak production) of mixed polyhalogenated paraffins (brominated-chlorinated paraffins, referred to as BCPs or polyhalogenated alkanes, PXAs) have also been manufactured for use as flame retardants in commercial materials such as PVC, polyurethane foam, textiles, etc. [5,6].

Conventionally, CP manufacturers characterise their products as short-, medium-, and long-chain CPs (SCCPs, MCCPs, and LCCPs, respectively) based on the length of the carbon chain ($C_{10\text{-}13}$, $C_{14\text{-}17}$, and traditionally $C_{18\text{-}30}$, respectively, although literature may also refer to the latter as $C_{\geq 18}$, $C_{18\text{-}20}$ or $C_{>20}$). The degree of chlorination is influenced by the industrial applications of the products. Some longer chain LCCPs products which are increasingly being produced may be referred to as very long chain CPs (vLCCPs) [7]. Similarly, CPs with very short chains lengths (vSCCPs, typically, C_6 to C_9) have also been detected, both in abiotic and biotic media [8–12].

Historically, these chemical products were known under various names, e.g. chloraffins, chlorcosanes, chlorowaxes, until the more recently used term – chlorinated paraffins (CPs). Similarly, the terms used for the analysis of polychlorinated alkanes (PCAs, usually with carbon chain lengths of $C_{\geq 10}$), initially for assaying manufactured products and subsequently for estimating occurrences in environmental and biological samples, have also varied. Despite representing two distinct although mutually related chemical mixtures, the terms CPs and PCAs are used synonymously for reporting occurrences, generally without clarification despite clearly being directed to the estimation of PCAs. The terms widely used for describing the mixtures e.g., SCCP, MCCP, etc. are also indistinct because the manufactured products were/are based on the intended applications and contain varying proportions of different chain length PCAs [9,13,14] even if the terms specify a range of carbon lengths. For example, LCCP products, which are specified as containing chain lengths of $C_{\geq 18}$ have been shown to contain as much as 52 % C_{17}-MCCPs [15]. Other ambiguities can arise through the terms used for identifying and reporting estimated PCA occurrences. An individual PCA is sometimes referred to as a constitutional isomer despite the IUPAC definition of this term specifying that it refers to individual compounds that show "isomerism between structures differing in constitution and described by different line formulae e.g. CH_3OCH_3 and CH_3CH_2OH" [16]. Another example is the reporting of measured PCAs as total CPs or total CP mixtures (e.g., total SCCPs), despite the very poor, or no instrument response to PCAs with one to four chlorines [4,17–19] or to some PCAs with terminal chlorines [15]. The exclusion of these elements clearly invalidates the use of "total" in the reported occurrences. This ambiguity in the terms used for describing PCAs and reporting measured occurrences can lead to misinterpretation of the data, not only between analytical chemists but also between professionals in disciplines that generate or use PCA data, such as toxicology, risk assessment and regulatory science.

Chemically, the products targeted during CP manufacture are the PCAs, typically with carbon chain lengths of $C_{\geq 10}$ and the general empirical formula of $C_nH_{2n+2\text{-}x}Cl_x$. The most common production methods used direct chlorination of crude *n*-alkane feedstocks using chlorine, until the required level of chlorination was achieved [14,20]. Additives may be introduced in order to maintain mobility in the higher chlorinated products [1,20]. In addition to PCAs, unreacted alkanes, chlorinated alkenes (polychlorinated alkenes, commonly referred to as polychlorinated olefins), polychlorinated branched chain or polychlorinated iso-alkanes, added stabilizers and in some cases, chlorinated fatty acid methyl esters, also form part of the CP product [9,21,22]. Other reported by-products such as polychlorinated biphenyls (PCBs), polychlorinated naphthalenes (PCNs) and polychlorinated dibenzo-*p*-dioxins and furans (PCDD/Fs) are minor but toxicologically significant components [23,24]. Production using linear alpha-alkenes has also been applied commercially and $C_{12\text{-}24}$ chlorinated alkenes were registered in the USA, Europe, China and Japan, but the actual products were PCAs (although these are no longer in the current Toxic Substances Control Act or REACH inventories) [25].

CP products contain PCAs with varying numbers of chlorine atoms per molecule, depending largely on the applied level of chlorination. Higher levels of chlorination yield products with a larger proportion of more highly chlorinated PCAs, which includes the possibility of multiple chlorines per carbon [14]. However, most methods of assay and measurement are based on the pragmatic concept that the carbons in the chlorinated alkane chains bear no more than a single chlorine (Fig. 1). This is a practical but also reasonable assumption because the chlorination of an alkyl carbon atom reduces the activity of the hydrogen atoms on the adjacent carbons, deactivating vicinal chlorine substitution, particularly when other substitution positions are available [1,26]. However, multiple chlorine (geminal) substitution on alkyl carbons can occur and is dependent on the prevailing thermodynamics such as the temperature and the level of solvation [27]. This is possible in highly chlorinated commercial CP mixtures as has been reported on terminal as well as vicinal carbons [9,15,28].

One of the major challenges in characterising the composition of PCAs, whether in the original products or once dispersed in the environment, arises from the very high numbers of individual compounds that are formed during production. As it is not yet possible to separate these by any technique and define the constituents, some studies have estimated theoretical numbers of individual PCAs. Assuming a single chlorine per carbon of linear alkanes, the formula $C_nH_{2n+2\text{-}x}Cl_x$, would theoretically yield 4159 isomeric compounds for a chain length of C_{13} and 536,887,295 for C_{30} [29,30]. On the other hand, a wider estimation that includes the possibility of multiple chlorination per carbon as well as chirality (all the non-terminal carbons in linear alkanes are pro-chiral so two forms, *r* and *s*, per substituted carbon are possible), reveals that 67,108,864 individual PCAs for a C_{13} chain are theoretically possible [14]. In reality, the actual number formed during production is likely to be considerably smaller [14,28], as can be seen from the examples of other complex chemical products such as congener mixtures of polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs) or toxaphenes where only 50–60 %, 29 % and 4 %, respectively of the theoretical number of compounds have been reported in commercial products [14,31,32]. Accordingly, Vetter et al. [14], predicted an occurrence of 32,000 individual compounds for the C_{13} example described above, assuming only 0.1 % of the theoretical abundance and no stereoisomerism. However, each additional carbon results in up to a four-fold increase in numbers, so for manufactured products containing chain lengths from C_{10} to at least C_{35}, the projected number of individual PCAs is immense [30].

In addition to this numerical complexity there are other difficulties in characterising PCA occurrences. The composition of commercial mixtures or analytical standards can be estimated in order to provide proportionate chain-length data but as the environmental and biological lability of individual compounds is not known, the partial characterisation of the standard which is used to construct quantitative models is unlikely to match the actual occurrence in sample matrices. It is clear that the composition of commercially produced CPs undergoes changes which can occur during application [21], followed by further changes through environmental transformation processes. These may be abiotic – such as photo-ionisation [33], selective evaporation of more volatile components [34], selective partitioning between different compartments [35,36], or biotic – e.g., microbial transformations [37–39] or selective uptake by plants [40,41]. The composition is further modified

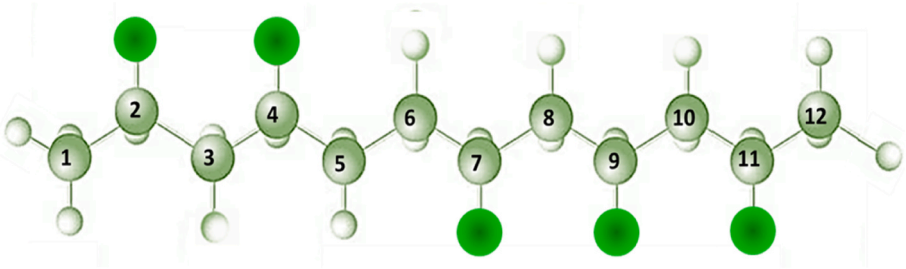

Fig. 1. Conventional labelling of a C_{12} PCA – 2,4,7,9,11-pentachlorododecane (2,4,7,9,11-$C_{12}H_{21}Cl_5$).

by animals and ultimately, humans, either through selective uptake and/or metabolism [42–46]. Thus, as described earlier [47,48], the resulting patterns of PCA occurrence in animal or human tissues will differ from the manufactured CP products. This leads to another difficulty in characterising PCAs because most analytical quantitation models assume that the profile of the standards used will match that of the sample which is unlikely following environmental and metabolic processes.

There have been increasing efforts to phase out SCCPs since the late 1990s [49] and latterly, MCCPs as well [50,51]. These culminated in a global restriction on SCCPs in 2017 when they were listed in Annex A (elimination of production and use) of the Stockholm Convention [52] as Persistent Organic Pollutants (POPs). There still remain a number of exemptions, including use as a secondary plasticizer in PVC (although not for toys or other children's products). These exemptions, for SCCPs and also for MCCPs as new candidate substances, have recently been reviewed [51,53], and the European Chemicals Agency (ECHA) is in the final stages of proposed regulation of MCCPs [54].

This article proposes descriptors and abbreviations for the terms used in the study of PCAs in an effort to harmonise reported results and reduce ambiguity for all users of PCA data. The basic assumptions made in these descriptions are that PCAs refer to linear chlorinated alkanes with one chlorine per carbon atom.

2. Descriptive terms for polychlorinated alkanes (PCAs)

2.1. Individual PCAs and configurational isomers

Individual polychlorinated alkanes (PCAs) are compounds with the generic formula $C_nH_{2n+2-x}Cl_x$, which corresponds to a *n*-alkane molecule with a carbon chain length of n and x number of chlorine substituents. Conventionally, n ranges from 10 to 32, although PCAs with chain lengths of $C_{32\text{-}48}$ have been reported in sediments, dust or hand wipes [11,55–57]. Additionally, PCAs with chain lengths of C_6 to C_9 have been reported in various biological and abiotic media and in standard mixtures [8,11,55,58] including those registered as products (e.g. a C_6–C_{18} mixture, CAS Number 68920-70-7). It is currently not possible to separate and measure individual PCA concentrations in any CP mixture but a number of analytical standards are available. Individual PCA standards are very useful tools that help to characterise the behaviour of PCAs in a variety of circumstances, e.g. during mass spectrometric (MS) ionisation, lability to microbial treatment and metabolism, etc. [37,38]. In more general terms, all individual PCAs, irrespective of chain length or the number of chlorines per molecule are referred to as **PCA congeners**.

The variable distribution of chlorine atoms on an individual PCA congener with specified values for n and x gives rise to a number of isomeric forms depending on the values and on the configuration of the chlorine atoms. For example, if we consider the polychlorinated tridecanes, $C_{13}H_{27}Cl$ would theoretically have seven **configurational isomers**, $C_{13}H_{26}Cl_2$ would have 42 configurational isomers and so on, with the maximum number being seen for $C_{13}H_{22}Cl_6$ and $C_{13}H_{21}Cl_7$, with 868 configurational isomers each [29]. These isomers can be identified conventionally by the IUPAC rules on the numbering of haloalkanes based on the length of the alkane chain and the positions or configurations of the substituted chlorine atoms as shown for 2,4,7,9,11-pentachlorododecane in Fig. 1.

2.2. PCA stereoisomers

The current state of knowledge does not allow any characterisation of PCAs with respect to their chirality, though it is worth noting that all non-terminal carbons are inherently prochiral. Substitution with a chlorine atom on any of these carbons would lead to a stereocentre, generating two chiral forms of the molecule per stereocentre. So, for example, 2,4,6,8,9,10-hexachlorinated tridecane would present six stereocentres, which would lead to 2^6 or 64 potential **PCA stereoisomers**.

2.3. PCA isotopologues and isotopomers

The abundance of the natural stable isotopes, ^{35}Cl (75.77 %) and ^{37}Cl (24.23 %) of the chlorine atoms on PCA molecules, gives rise to distinct molecular entities that have the same molecular formula but differ in the isotopic composition of chlorine as seen in the example where $C_{12}H_{18}^{35}Cl_5^{37}Cl_3$ is distinct from $C_{12}H_{18}^{35}Cl_4^{37}Cl_4$. These entities are referred to as **isotopologues** and occur in defined relative abundances for a particular PCA congener. As MS measurements of PCAs are complex with a multitude of ions or transitions that are generated during the ionisation process, mass to charge (*m/z*) discrimination between isotopologues is exploited to provide confirmation of the identity of a particular PCA or for a group of configurational isomers.

Isotopically labelled individual reference standards that are produced for PCA analysis in which either the ^{12}C atoms are replaced by ^{13}C or the ^{1}H atoms are replaced by deuterium would also be considered as isotopologues albeit with a different analytical purpose.

A PCA group of configurational isomers that can all exist in the same isotopologue form, e.g., 2,4,6,8,9,10-$C_{12}H_{20}^{35}Cl_4^{37}Cl_2$, 3,4,5,9,10,11-$C_{12}H_{20}^{35}Cl_4^{37}Cl_2$, 2,3,5,7,9,11-$C_{12}H_{20}^{35}Cl_4^{37}Cl_2$, etc. are all referred to as **isotopomers** of hexachlorododecane – $C_{12}H_{20}Cl_6$. As it is not currently possible to separate configurational isomers within a PCA group, the collective signal from an isotopomer group can be used for the purposes of quantitation or qualification during MS analysis.

2.4. PCA homologue groups – specified by chain length and by chain length including chlorine number

One of the practical outcomes of the inability to separate individual PCAs is that the estimated concentrations or amounts need to be expressed collectively either as the sum of all measured PCAs or as a subset of the sum. The ambiguity resulting from the use of older descriptors such as SCCPs can be overcome through the use of the sum of all measured PCAs within a range of chain lengths, e.g. PCA-$C_{10\text{-}13}$. Additionally, it is also useful to express measured concentrations as the sum of all PCAs within a particular chain length as this provides more specific information. This sum of all PCA congeners within a specified chain

length would include all the configurational isomers for all of the possible levels of chlorination of the chain, i.e. all of the PCA congeners within a specified **chain length e.g., C_{10}**. Based on historical and current production, these summed PCA values would typically include individual homologue groups of chlorinated chain lengths from C_{10} to C_{32}. However, as noted earlier, the occurrence of PCAs with carbons chain lengths that are outside this range (C_6 to C_9 and $C_{>32}$) have been reported in commercial mixtures and in environmental samples, so data on these chain lengths would add to the characterisation of production and occurrence.

Homologues of a particular chain length C_n can be further differentiated by specifying the number of chlorines that are present on the chain, i.e. C_nCl_1 to C_nCl_x, which in the case of C_{10} would result in ten **homologue groups**, specified by chain length as well as chlorine number, eleven homologue groups in the case of C_{11}, and so on. These homologue groups, composed of all the configurational isomers for a specified carbon chain length and chlorine number are particularly useful in describing the PCA pattern of occurrence in a particular environmental or biota sample or in a standard. As it is not possible to separate and measure individual PCA congeners as yet, these homologue groups currently represent the most specific level at which PCA occurrence can be characterised.

Additional homologue groups (e.g., C_nCl_{n+1}) are possible in case of multiple chlorination which occurs when a higher intensity of chlorination is applied during production and can result in more than one chlorine per carbon. The extent of multiple chlorination would vary depending on the intensity of the chlorination process and theoretically could reach C_nCl_{2n+2} (perchlorinated alkanes, at least up to C_6Cl_{14} are known and have been studied - [59]), but in practice the extent would be limited by the utility and physical characteristics of the product. In reality, the occurrences of C_nCl_{n+1} and C_nCl_{n+2} have been reported in abiotic matrices such as dust, soil and sediments [7] and the presence of -CCl_2-and -CCl_3-groups have been reported in commercial CP products [9,15], so a limited amount of multiple chlorination has been evidenced. Multiple chlorination of carbon atoms imposes additional complexity to characterising PCAs as it is not currently possible (without using NMR techniques) to identify whether, for example a $C_{14}Cl_7$ homologue group could conventionally contain 2,3,5,7,9,10,11-heptachlorotetradecane or unconventionally, 1,1,3,5,5,10,13-heptachlorotetradecane. The reported occurrences of multiple chlorination should be further investigated by matrix type so that they can be contextualised to risk – i.e., is the additional occurrence quantitatively significant, particularly in biota, food, animal tissues and is it consequently, toxicologically relevant to human exposure? It is therefore important that occurrences of multiple chlorination are appropriately (i.e., identified as a multiple chlorinated homologue group) included with the conventional homologue groupings.

3. Terms used for reporting of PCA occurrence

3.1. Sum (Σ) of measured PCAs

One of the most important elements of the risk assessment of PCAs is data on the occurrence of these contaminants in food and the environment. The last few years have seen an increase in the number of reported data, concurrent with the advances made in instrumentation and very recently, in the availability of newer analytical standards. Harmonisation and consistency of the manner in which these data are reported would allow easier comparability and complementarity between data sets, and thus avoid misunderstanding between research findings and aid risk evaluation and management.

Unlike current studies, much of the historical PCA literature reported occurrences, either as the sum of all measured PCAs or as the sum of chain length mixtures, e.g. C_{10}–C_{13} (SCCPs) or C_{14}–C_{17} (MCCPs). For practical reasons, i.e., inadequate instrument response and the poor availability of standards, longer chain ($C_{\geq 18}$) data were rarely reported. These summed concentrations have therefore represented the PCA congeners that were measurable in the sample or standard, i.e., the sum of the configurational isomers within the homologue groups present in a chain length mixture, or the sum of all measured PCAs. This sum of measured congeners continues to be reported in current literature although it is increasingly used to represent concentrations of homologue groups within a PCA chain length as well as the sum of a specified chain length mixture or the sum of all measured PCAs in the sample.

It is important to acknowledge that the concentrations or amounts of PCAs reported are the sum of measured congeners within a homologue group, or the collective sum representing all the measured homologue groups and chain lengths, as opposed to the total PCAs present in a sample. It is not currently possible to include all the PCA congeners present in a sample, as is implied by the term "total PCA". The lack of response to some PCA configurations even with the use of current instrumentation cannot confirm the absence or proposed lower abundance of these configurations at concentrations that can realistically be expected to occur for example, in foods (ranging from sub-ng g^{-1} to low μg g^{-1} levels). Commonly, this lack of response is seen for all PCAs with one to four chlorines and those with terminal chlorine substitution [4,15,17–19]. Additionally, as there are no individual PCA standards that cover all possible configurations, it is not possible to specify the full set of unresponsive PCA congeners. To some extent, PCAs with very poor response may be compensated for in quantitation routines, but this would be based on the information that ultimately comes from the response of the analytical instrument to individual PCA standards or to standard mixtures that cannot be fully speciated.

Thus, "total PCA concentration" is currently an unquantifiable term. Instead, what is reported is actually the "**sum of measured PCAs**" and is a more realistic representation of the concentration or amount in a given sample. The PCAs included in this sum should be specified in the description of the analytical methodology used for measurement.

3.2. Sum of PCAs by carbon chain length and by homologue group

Depending on the sophistication of the available methodology and instrumentation, PCAs can be reported as the sum of congeners, within a specified carbon **chain length congener group - ΣPCAs-C_n**, e.g., ΣPCAs-C_{12}, or as the sum of conventional groupings, e.g., **ΣPCAs-$C_{10\text{-}13}$, ΣPCAs-$C_{14\text{-}17}$, ΣPCAs-$C_{18\text{-}20}$, ΣPCAs-$C_{21\text{-}32}$** or as the sum of all measured chain lengths that the applied methodology is capable of, **ΣPCAs-$C_{a\text{-}z}$** where C_a could represent C_{10} or a smaller carbon chain length and C_z could represent up to C_{32} or a higher chain length depending on the capability of the instrumentation and the measured occurrence in a sample.

Similarly, depending on the capability of the instrumentation used, an increasing number of recent studies have also reported PCA concentrations more specifically, using the sum of measured configurational isomers or homologue group e.g., **ΣPCAs-$C_{10}Cl_6$**. As mentioned earlier, this level of specificity is desirable as it provides an indication of which homologues dominate in a particular sample. Additionally, the reporting of the sum of homologue groups provides data that is independent of which commercial mixtures were produced and used or the extent to which PCAs are environmentally or biologically modified. However, as recently noted, a larger number of reliable homologue group standards are required in order to allow better quantitation of this parameter.

Reporting of PCAs by the sum of homologue groups also allows a greater measure of comparability between data and provides an indication of which PCAs are more persistent and environmentally relevant. This can be conveniently visualised through the use of **PCA homologue group patterns** as shown in Fig. 2. Here, the dominant PCAs in the mean of urban/rural air samples (n = 16, measured using APCI-qToF-HRMS) are seen to be C_9Cl_5 and C_9Cl_6, in comparison to the mean for fish tissue (n = 19, measured using GC-ECNI-Orbitrap-HRMS), where $C_{14}Cl_8$ and $C_{14}Cl_9$ are seen as predominating. In order to increase the comparability between different sets of data, simple forms of presentation generated

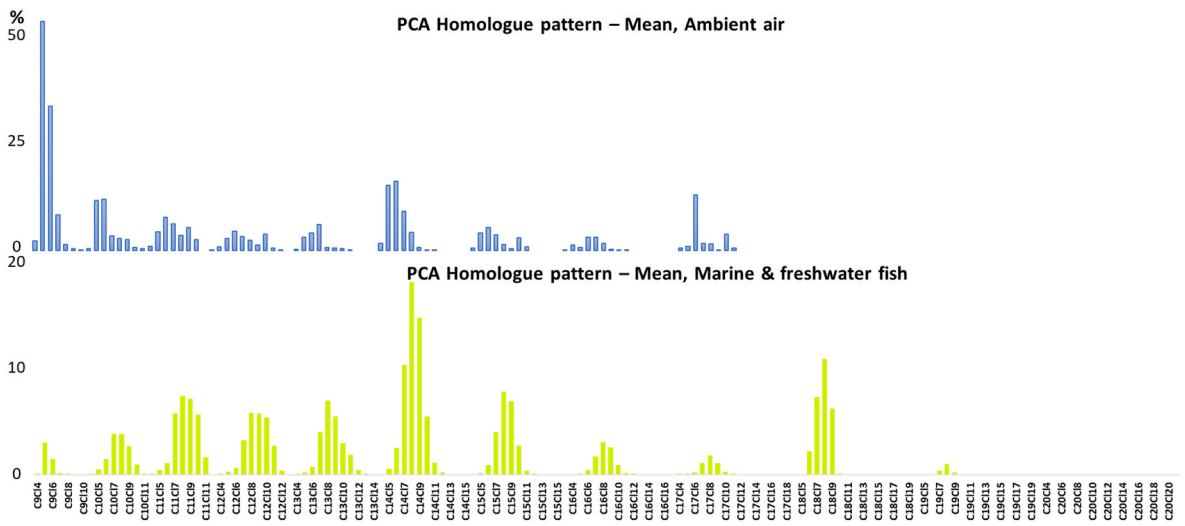

Fig. 2. Simplified visualisation of PCA homologue group patterns allows easier comparability of occurrence. Here, a mean pattern derived from urban and rural air (n = 16) shows a predominance of shorter carbon chain lengths as well as lower chlorinated homologue groups when compared to fish tissues (n = 19).

through the use of commonly used software (e.g. MS Excel based charts are used in Fig. 2), and a standardised range of homologues (e.g. $C_{10}Cl_5$ to $C_{17}Cl_{12}$ are commonly reported for GC-MS measurements while studies using LC-MS report $C_{10}Cl_4$ to $C_{20}Cl_{12}$) would be accessible to a wider range of users.

However, the results of comparing patterns between different studies should be considered as indicative, rather than absolute. This is because PCA homologue group patterns can be influenced by the type of instrumentation used for measurement, the analytical standards and also the quantitative approach that is used to estimate group concentrations. The process of comparison would therefore be considerably aided if these and other relevant parameters were specified when homologue group patterns are presented.

The recommended terms and abbreviations for the parameters used to describe and express the occurrence of PCAs are listed in Table 1.

4. Discussion

It is important to present and discuss chemicals based on their correct (and where defined, IUPAC-based) chemical names. Also, as the ability to characterise occurrences has improved significantly, it is important to make a clear distinction between CPs and PCAs. Both identifications,

Table 1
Summary of recommended polychlorinated alkane (PCA) descriptors and abbreviations.

Polychlorinated alkanes (PCAs): Descriptors and Recommended Abbreviations			
Term	Descriptor, Abbreviation	Example	Synonyms or historical terms
Chlorinated Paraffins - Commercial Product	**CPs**	Witaclor 149, Cereclor 60L	Chloraffins, Chlorcosanes, Chlorowaxes
Chlorinated Paraffins - analytically determined concentration or quantity	**Polychlorinated alkanes, PCAs**		CPs
Individual PCA or PCA congener	Generic formula $\mathbf{C_nH_{2n+2-x}Cl_x}$	$C_{11}H_{18}Cl_6$, $C_{14}H_{21}Cl_9$	isomers
Isomeric forms of PCAs	**Configurational isomer**	2,3,6,8,10-pentachlorododecane	constitutional isomer
Chiral forms of PCAs	An individual congener may have a number of **PCA stereoisomers**	2*S*,4*S*,6*R*,8*R*-tetrachloroundecane, 2R,4*R*,6*R*,8*R*-tetrachloroundecane	
PCAs with the same molecular formula but different isotopic composition	**Isotopologues**	$C_{12}H_{18}^{35}Cl_5^{37}Cl_3$ and $C_{12}H_{18}^{35}Cl_4^{37}Cl_5$	
Configurational isomers with the same isotopologue composition	**Isotopomers**	2,4,6,8,9,10-$C_{12}H_{20}^{35}Cl_4^{37}Cl_2$, 3,4,5,9,10,11-$C_{12}H_{20}^{35}Cl_4^{37}Cl_2$, 2,3,5,7,9,11-$C_{12}H_{20}^{35}Cl_4^{37}Cl_2$	
All PCA congeners within a specified carbon chain length	**Chain length congener group**	PCAs–C_{10}, PCAs–C_{18}	
All PCA congeners with the same molecular formula (configurational isomer group)	**Homologue group**	PCAs–$C_{12}Cl_6$, PCAs–$C_{13}Cl_7$, PCAs–$C_{18}Cl_9$, etc.	
[a]Measured sum of PCA congeners within a specified carbon chain length	Sum of congeners of specified carbon chain length **ΣPCAs-C_n**	e.g., ΣPCAs-C_{13}	
[a]Measured sum of PCA congeners within a range of specified carbon chain lengths (includes conventionally reported groups)	**ΣPCAs-$C_{6\text{-}9}$**, **ΣPCAs-$C_{10\text{-}13}$**, **ΣPCAs-$C_{14\text{-}17}$**, **ΣPCAs-$C_{18\text{-}20}$**, **ΣPCAs-$C_{18\text{-}32}$**		Sum of short, medium and long chain CPs, or SCCPs, MCCPs, LCCPs
Sum of all [a]measured PCA congeners for all specified carbon chain lengths	**Sum of all measured PCAs**, **ΣPCAs-$C_{a\text{-}z}$**	ΣPCAs-$C_{10\text{-}21}$	Total CP
[a]Measured sum of configurational isomers with the same molecular formula	**Homologue group sum**	ΣPCAs-$C_{10}Cl_7$	
Graphical presentation of measured homologue group concentrations in a sample (estimated mass fraction)	**Homologue group pattern**	See Fig. 2	

Note.
[a] As defined by the capability of the analytical method used.

CPs or PCAs, are pertinent to the circumstances in which they are used. For example, in the listing by the Stockholm Convention on POPs, the term CPs (or specifically, SCCPs which are listed and MCCPs which are proposed) is appropriate as the eventual objective is to terminate or severely restrict the manufacture of the product. On the other hand, the vast majority of studies that report occurrence, behaviour and effects, use methodology that is focussed solely on the analysis of PCAs, although some acknowledge the presence of by-products in CP mixtures [14,21,22,60]. The distinction is particularly relevant for toxicology and risk assessment purposes because as mentioned earlier, the composition of PCAs in CP products is likely to be different to the residual composition that humans and animals are exposed to Fernandes et al. [47,48], both, in terms of the PCA profile as well as the fate of the by-products. The focus of analytical methodologies, toxicological studies, risk assessment and fate on PCAs rather than CPs would seem appropriate as it could be justified on the basis of.

- PCAs are by far the largest component of commercial CP mixtures,
- other significant by-products such as the polychlorinated alkenes (with single or multiple unsaturation) are chemically and metabolically more prone to transformation because of the reactivity of the pi-(π) bonding to chemical or enzymatic attack, which equates to higher environmental and metabolic lability [46], and
- toxicologically significant trace impurities such as PCBs, PCDD/Fs and PCNs are addressed by separate controls to reduce environmental and human exposure [52,61–63].

Other less significant components of commercial CP mixtures include unreacted alkanes as well as branched chain PCAs which may to some extent, be inadvertently included in quantitative estimates of PCAs, due to the similarities in chemical composition and structure [64]. Although branched chain PCAs would reasonably be expected as impurities, they are likely to be minor. One reason for this is that branched chain alkanes may be intentionally limited from the feedstock during production because their presence impairs the photo- and thermal stability of CP products and also causes discolouration [20,65].

The ultimate objective of determining PCAs in abiotic matrices, biota, foods and humans is to allow the estimation of human and environmental exposure and thus the risk to health arising through dietary and/or other adsorption pathways. The most recent attempt of a structured assessment of risk to human health [66] was unable to fulfil this task because of a lack of adequate supporting data on food occurrence or comprehensive studies on toxicological endpoints. The reasons for this shortfall arise directly from the historical inability to characterise PCA occurrence due to analytical capability, appropriate, reliable and authentic chemical standards and guidance on which PCAs were more relevant (apart from the relatively indistinct indication that SCCPs should be targeted). Analytical methodology, aided by improvements in the capability of MS methods has advanced significantly to a stage where the occurrence of a range of PCA homologue groups and specified carbon chain lengths can be identified in environmental, food and human tissue samples. The issue of reliability and commercial availability of a range of analytical standards was recently identified [15,67,68] and newer standards of individual PCAs, single chain length PCAs and homologue group have recently, or will imminently, become available [69–71].

It is unlikely in the foreseeable future that PCA characterisation beyond the specificity of homologue groups would be possible without significant advances e.g., in separation techniques. Thus, the level of guidance for future toxicological and risk studies would rest with characterisation of the occurrence of PCA homologue groups in dietary and other sources of human exposure. There is a circularity in this process in that future toxicology that is guided by occurrence data as well as the availability of reliable standards would be able to refine the selection of risk relevant PCAs for analytical determination.

In addition to the analytical difficulties in measuring PCAs, other factors such as the variety of commercial mixtures that have been produced and used globally and the multiplicity of carbon chain lengths and homologue groups, give the reporting of PCA occurrences a greater complexity than that of other POPs including those comprised of a number of congeners. The use of different terminology for the same parameter or sets of parameters could lead to misunderstanding or to misinterpretation of reported data. It is therefore important to ensure that the results of PCA measurement are reported appropriately with relevant and harmonised terminology, in order to minimise ambiguity to subsequent users (e.g., exposure and risk assessment and management, regulation, etc.) of the data.

5. Conclusions and future considerations

Environmental and analytical chemistry play an important role in characterising pollutant occurrences and elaborating their physicochemical properties. The findings of diverse studies by multiple research groups covering different aspects of the behaviour of PCAs have been rationalised in order to recommend harmonised nomenclature of terms and abbreviations for these chemicals as has been done for other similar pollutants such as organophosphate flame retardants, per- and polyfluoroalkyl substances, and plasticizers [72,73]. The underlying objective of this joint effort on how to deal with the vast group of PCAs and their commercial products (CPs) was to avoid misunderstanding by all users of the data. In addition to using a common set of terminology to represent PCAs, those generating and using the data should note that.

- The “Sum of measured PCAs” (i.e. ΣPCAs, ΣPCAs-$C_{a\text{-}z}$) provides a proper representation of the estimated concentration or amount of PCAs in a given sample. The reporting of a PCA quantitation as “total” PCA concentration is currently inaccurate and must be avoided.
- It is important to report the sums of individual chain lengths, e.g., ΣPCAs-C_{10}, ΣPCAs-C_{11}, ΣPCAs-C_{12}, etc., and where quantified, the sums of homologue groups. This would allow future toxicological studies and risk assessment to consider different combinations of PCAs based on occurrence and biological effects.
- Although the current focus of quantitative PCA estimation is very much on the sum of congeners within chain lengths and homologue groups, it is important to maintain studies on the chemical, environmental and metabolic behaviour of a wide and varied range of individual congeners. This information would allow a more refined characterisation in relation to the adsorption, disposition, metabolism and excretion (ADME) behaviour of PCAs
- For relevant biological matrices (e.g. blood serum, breast milk, adipose tissue, etc.), the reporting of PCA concentrations on a wet and lipid weight basis (or reporting of the sample lipid content) would aid the comparison of exposure data between studies and contextualise simultaneous contamination from other POPs.

The field of CP analysis presents a complex spectrum that is gradually being explored and elucidated with the emergence of new findings. The recommended terms suggested here may therefore need to be extended in future in order to assimilate the increasing knowledge. One of the limitations of the scope of this article is the conventional definition of PCAs with one chlorine per carbon. This is supported by the chemistry of formation under normal conditions, but a higher intensity of chlorination during production can result in multiple chlorines per carbon. The extent of multiple chlorination should be further investigated by matrix type so that any additional risk can be evaluated, i.e., through the qualitative and quantitative significance of these additional homologue groups combined with the extent to which they occur in matrices that are relevant to human exposure.

Another set of products that may need to be considered for future inclusion are the PXAs. Although reported production of these is comparatively very small, the US Toxic Substances Control Act (TSCA)

inventory showed an increase from 109 to 245 t/year from 2016 to 2019 for CAS 68527-01-5 [74]. As far as is currently known, information on the extent of occurrence, toxicology and risk to human health is either unavailable or limited.

Credit statement

A. Fernandes: Conceptualization and initiation (equal); Writing – Original Draft Preparation (lead); Writing – Review & Editing (lead). K. Krätschmer: Writing – Original Draft Preparation (supporting); Writing – Review & Editing (equal). B. Yuan, T. McGrath: Writing – Review, Editing and Draft (supporting). R. Letcher, R. Cariou, J. Mueller, D. Muir, G. Yu, T. Wang, W. Vetter, B. Martinus, S. Brandsma: Writing – Review & Editing (supporting). Å. Bergman: Conceptualization and initiation (equal); Writing – Original Draft Preparation (supporting); Writing – Review & Editing (equal).

Declaration of competing interest

The authors assert that they have no conflict of interest (financial or non-financial) in the subject matter discussed in this manuscript.

Data availability

No data was used for the research described in the article.

References

[1] P. Howard, J. Santodonato, S. Saxena, Investigation of Selected Potential Environmental Contaminants, Chlorinated Paraffins. U.S. Environment Protection Agency. Document No. EPA-560/2 -75-007, National Technical Information Service, Springfield, Virginia, 1975, p. 22151. USA.

[2] C. Chen, A. Chen, F. Zhan, F. Wania, S. Zhang, L. Li, J. Liu, Global historical production, use, stocks, and emissions of short-, medium-, and long-chain chlorinated paraffins, Environ. Sci. Technol. 56 (2022), 7895–7904.

[3] L. van Mourik, M. Brits, S. Brandsma, J. de Boer, Current status of analytical methods for chlorinated paraffins, Organohalogen Compd. 81 (2019) 360–362.

[4] L. van Mourik, C. Gaus, P. Leonards, J. de Boer, Recent developments in capabilities for analysing chlorinated paraffins in environmental matrices: a review, Chemosphere 136 (2015) 259–272.

[5] L. Chibwe, A. Myers, A. De Silva, E. Reiner, K. Jobst, D. Muir, B. Yuan, C12−30 α-bromo-chloro "alkenes": characterization of a poorly identified flame retardant and potential environmental implications, Environ. Sci. Technol. 53 (2019) 10835–10844.

[6] C. He, L. Van Mourik, S. Brandsma, P. Thai, X. Wang, S. Chen, K. Thomas, J. Mueller, Semiquantitative characterization of bromo-chloro paraffins and olefins in the Australian environment, Environ. Sci. Technol. 56 (17) (2022) 12452–12459.

[7] B. Yuan, H. Rüdel, C.A. de Wit, J. Koschorreck, Identifying emerging environmental concerns from long-chain chlorinated paraffins towards German ecosystems, J. Hazard Mater. 424 C (2022), 127607.

[8] Y. Zhou, C.A. de Wit, G. Yin, X. Du, B. Yuan, Shorter than short-chain: very short-chain chlorinated paraffins (vSCCPs) found in wildlife from the Yangtze River Delta, Environ. Int. 130 (2019), 104955.

[9] J. Sprengel, W. Vetter, NMR and GC/MS analysis of industrial chloroparaffin mixtures, Anal. Bioanal. Chem. 412 (2020) 4669–4679, https://doi.org/10.1007/s00216-020-02720-7.

[10] B. Yuan, M.S. McLachlan, A.M. Roos, A. Strid, C.A. de Wit, Long-chain chlorinated paraffins have reached the arctic, Environ. Sci. Technol. Lett. 8 (9) (2021) 753–759.

[11] B. Yuan, J.H. Tai, J.A. Padilla-Sánchez, E. Papadopoulou, L. Småstuen Haug, C. A. de Wit, Human exposure to chlorinated paraffins via inhalation and dust ingestion in a Norwegian cohort, Environ. Sci. Technol. 55 (2) (2021) 1145–1154, https://doi.org/10.1021/acs.est.0c05891.

[12] L. Ding, S. Zhang, Y. Zhu, N. Zhao, W. Yan, Y. Li, Overlooked long-chain chlorinated paraffin (LCCP) contamination in foodstuff from China, Sci. Total Environ. 801 (2021), 149775.

[13] T. Li, S. Gao, Y. Ben, H. Zhang, Q. Kang, Y. Wan, Screening of chlorinated paraffins and unsaturated analogues in commercial mixtures: confirmation of their occurrences in the atmosphere, Environ. Sci. Technol. 52 (2018) 1862–1870, https://doi.org/10.1021/acs.est.7b04761.

[14] W. Vetter, J. Sprengel, K. Krätschmer, Chlorinated paraffins – a historical consideration including remarks on their complexity, Chemosphere 287 (1) (2022), 132032, https://doi.org/10.1016/j.chemosphere.2021.132032.

[15] A. Fernandes, W. Vetter, C. Dirks, L. van Mourik, R. Cariou, J. Sprengel, N. Heeb, A. Lentjes, K. Krätschmer, Determination of chlorinated paraffins (CPs): analytical conundrums and the pressing need for reliable and relevant standards, Chemosphere 286 (2022), 131878.

[16] IUPAC, Compendium of chemical terminology, in: (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson, second ed., Blackwell Scientific Publications, Oxford, 2019 https://doi.org/10.1351/goldbook, 1997). Online version (2019-) created by S. J. Chalk. ISBN 0-9678550-9-8.

[17] B. Yuan, D. Muir, M. MacLeod, Methods for trace analysis of short-, medium-, and long-chain chlorinated paraffins: critical review and recommendations, Anal. Chim. Acta 1074 (2019) 16–32.

[18] M. Mézière, K. Krätschmer, I. Pērkons, D. Zacs, P. Marchand, B. Le Bizec, A. Schächtele, R. Cariou, W. Vetter, Addressing main challenges regarding short- and medium-chain chlorinated paraffin analysis using GC/ECNI-MS and LC/ESI-MS methods, J. Am. Soc. Mass Spectrom. 31 (9) (2020) 1885–1895.

[19] M. Mézière, R. Cariou, F. Larvor, E. Bichon, Y. Guitton, P. Marchand, G. Dervilly, B. Le Bizec, Optimized characterization of short-, medium, and long-chain chlorinated paraffins in liquid chromatography-high resolution mass spectrometry, J. Chromatogr. A 1619 (2020), 460927.

[20] V. Zitko, Chlorinated paraffins, in: O. Hutzinger (Ed.), The Handbook of Environmental Chemistry Part 3A, Springer-Verlag, Berlin, 1980, pp. p149–p156, 1980, ISBN 978-3-662-15998-9.

[21] L. Schinkel, S. Lehner, M. Knobloch, P. Lienemann, C. Bogdal, K. McNeill, N. V. Heeb, Transformation of chlorinated paraffins to olefins during metal work and thermal exposure–Deconvolution of mass spectra and kinetics, Chemosphere 194 (2018) 803–811.

[22] Y. Sun, H. Cui, T. Li, S. Tao, J. Hu, Y. Wan, Protein-affinity guided identification of chlorinated paraffin components as ubiquitous chemicals, Environ. Int. 145 (2020), 106165.

[23] Å. Bergman, A. Hagman, S. Jacobsson, B. Jansson, M. Ahlman, Thermal degradation of polychlorinated alkanes, Chemosphere 13 (1984) 237–250.

[24] T. Takasuga, T. Nakano, Y. Shibata, Unintentional POPs contamination in chlorinated paraffins and related impacted chlorinated paraffin (CPs) – issues on impurities in high production volume chemicals, J. Environ. Chem. 23 (2013) 115–121.

[25] US EPA (U.S. Environmental Protection Agency), List of Toxic Chemicals within the Polychlorinated Alkanes Category and Guidance for Reporting, US Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, 1999, p. 14. EPA 745-B-99-023.

[26] W. Vaughan, F. Rust, The high-temperature chlorination of paraffin hydrocarbons, J. Org. Chem. 5 (5) (1940) 449–471.

[27] A.S. Bratolyubov, Principal factors in the free-radical chlorination of alkanes, Russ. Chem. Rev. 30 (11) (1961) 602.

[28] B. Yuan, D. Lysak, R. Soong, A. Haddad, A. Hisatsune, A. Moser, S. Golotvin, D. Argyropoulos, A.J. Simpson, D.C. Muir, Chlorines are not evenly substituted in chlorinated paraffins: a predicted NMR pattern matching framework for isomeric discrimination in complex contaminant mixtures, Environ. Sci. Technol. Lett. 7 (7) (2020) 496–503.

[29] G. Tomy, Analysis of chlorinated paraffins in environmental matrices: the ultimate challenge for the analytical chemist, in: J. de Boer, T. El-Sayed Ali (Eds.), Chlorinated Paraffins: Handb. Environ. Chem. 10, Springer, Heidelberg, London, 2010, pp. 83–106, 2010.

[30] Y. Zhou, B. Yuan, E. Nyberg, G. Yin, A. Bignert, A. Glynn, J.Ø. Odland, Y. Qiu, Y. Sun, Y. Wu, Q. Xiao, Chlorinated paraffins in human milk from urban sites in China, Sweden, and Norway, Environ. Sci. Technol. 54 (7) (2020) 4356–4366.

[31] G. Frame, J. Cochran, S. Bowadt, Complete PCB congener distributions for 17 Aroclor mixtures determined by 3 HRGC systems optimized for comprehensive, quantitative, congener-specific analysis, J. High Resolut. Chromatogr. 19 (1996) 657–668.

[32] M. La Guardia, R. Hale, E. Harvey, Detailed polybrominated diphenyl ether (PBDE) congener composition of the widely used penta-, octa-, and deca-PBDE technical flame-retardant mixtures, Environ. Sci. Technol. 40 (20) (2006) 6247–6254.

[33] I. Koh, W. Theimann, Study of photochemical oxidation of standard chlorinated paraffins and identification of degradation products, J. Photochem. Photobiol., A 139 (2–3) (2001) 205–215.

[34] Q. Ai, P. Zhang, L. Gao, X. Zhou, Y. Liu, D. Huang, L. Qiao, J. Weng, M. Zheng, Air–soil exchange of and risks posed by short- and medium-chain chlorinated paraffins: case study in a contaminated area in China, Chemosphere 297 (2022), 134230.

[35] W. Gao, J. Wu, Y. Wang, G. Jiang, Distribution and congener profiles of short-chain chlorinated paraffins in indoor/outdoor glass window surface films and their film-air partitioning in Beijing, China, Chemosphere 144 (2016) 1327–1333, https://doi.org/10.1016/j.chemosphere.2015.09.075.

[36] A. Jafarabadi, M. Dashtbozorg, E. Raudonytė-Svirbutavičienė, A. Bakhtiari, Chlorinated paraffins (SCCPs and MCCPs) in corals and water-SPM-sediment system in the Persian Gulf, Iran: a potential global threat for coral reefs, Environ. Pollut. 275 (2021), 116531.

[37] N. Heeb, S. Schalles, S. Lehner, L. Schinkel, I. Schilling, P. Lienemann, C. Bogdal, H. Kohler, Biotransformation of short-chain chlorinated paraffins (SCCPs) with LinA2: a HCH and HBCD converting bacterial dehydrohalogenase, Chemosphere 226 (2019) 744–754.

[38] M. Knobloch, F. Mathis, T. Fleischmann, H. Kohler, S. Kern, D. Bleiner, N. Heeb, Enzymatic synthesis and formation kinetics of mono-and di-hydroxylated chlorinated paraffins with the bacterial dehalogenase LinB from Sphingobium indicum, Chemosphere 291 (2022), 132939.

[39] L. Lyu, Y. He, C. Dong, G. Li, G. Wei, Z. Shao, S. Zhang, Characterization of chlorinated paraffin-degrading bacteria from marine estuarine sediments, J. Hazard Mater. 440 (2022), 129699.

[40] Y. Li, X. Hou, W. Chen, J. Liu, Q. Zhou, L. Schnoor, G. Jiang, Carbon chain decomposition of short chain chlorinated paraffins mediated by pumpkin and soybean seedlings, Environ. Sci. Technol. 53 (12) (2019) 6765–6772, https://doi.org/10.1021/acs.est.9b01215.
[41] X. Du, B. Yuan, J. Li, G. Yin, Y. Qiu, J. Zhao, X. Duan, Y. Wu, T. Lin, Y. Zhou, Distribution, behaviour, and risk assessment of chlorinated paraffins in paddy plants throughout whole growth cycle, Environ. Int. 167 (2022), 107404, https://doi.org/10.1016/j.envint.2022.107404.
[42] M. Castro, M. Breitholtz, B. Yuan, I. Athanassiadis, L. Asplund, A. Sobek, Partitioning of chlorinated paraffins (CPs) to Daphnia magna overlaps between restricted and in-use categories, Environ. Sci. Technol. 52 (17) (2018) 9713–9721, https://doi.org/10.1021/acs.est.8b00865.
[43] X. Du, B. Yuan, Y. Zhou, C.A. de Wit, Z. Zheng, G. Yin, Chlorinated paraffins in two snake species from the yangtze river delta: tissue distribution and biomagnification, Environ. Sci. Technol. 54 (5) (2020) 2753–2762, https://doi.org/10.1021/acs.est.9b06467.
[44] M. Mézière, P. Marchand, S. Hutinet, F. Larvor, E. Baéza, B. Le Bizec, G. Dervilly, R. Cariou, Transfer of short-, medium-, and long-chain chlorinated paraffins to eggs of laying hens after dietary exposure, Food Chem. 343 (2021), 128491.
[45] M. Mézière, P. Marchand, S. Hutinet, F. Larvor, E. Baéza, B. Le Bizec, G. Dervilly, R. Cariou, Accumulation of short-, medium-, and long-chains chlorinated paraffins in tissues of laying hens after dietary exposure, Food Chem. 351 (2021), 129289.
[46] P. Darnerud, Å. Bergman, Critical review on disposition of chlorinated paraffins in animals and humans, Environ. Int. 163 (2022), 107195.
[47] A. Fernandes, J. Falandysz, J. Olivero-Verbel, Editorial: a new focus on legacy pollutants: chlorinated paraffins (CPs) and polychlorinated naphthalenes (PCNs), Chemosphere 238 (2020), 124580.
[48] A. Fernandes, J. Falandysz, B. Yuan, Widening knowledge horizons on legacy POPs: chlorinated paraffins and polychlorinated naphthalenes, Chemosphere 289 (2022), 133131.
[49] OSPAR Commission, PARCOM Decision 95/1 on the Phasing Out of Short-Chained Chlorinated Paraffins, 1995. This measure has been set aside - see OSPAR 20/12/1, paragraph 9.22. Available at:.
[50] DEFRA (Department for Environment, Food & Rural Affairs, UK), Draft proposal to list chlorinated paraffins with carbon chain lengths in the range C14-17 and chlorination levels ≥45% chlorine by weight as a persistent organic pollutant (POP), Available at: https://www.gov.uk/government/publications/chlorinated-paraffins-with-carbon-chain-lengths-in-the-range-c14-17#full-publication-update-history, 2021.
[51] POPRC (United Nations Stockholm Convention POP Review Committee), 2022. Chlorinated paraffins with carbon chain lengths in the range C14–17 and chlorination levels at or exceeding 45 per cent chlorine by weight, Decision POPRC-18/4. Available at: https://chm.pops.int/TheConvention/POPsReviewCommittee/ReportsandDecisions/tabid/3309/ctl/Download/mid/26552/Default.aspx?id=41&ObjID=32205.
[52] Stockholm Convention, All POPs listed in the Stockholm convention, Available at: http://www.pops.int/TheConvention/ThePOPs/AllPOPs/tabid/2509/Default.aspx, 2019.
[53] POPRC (United Nations Stockholm Convention POP Review Committee), Review of Information Related to Specific Exemptions for Decabromodiphenyl Ether and SCCPs, Decision POPRC-18/6, https://chm.pops.int/TheConvention/POPsReviewCommittee/ReportsandDecisions/tabid/3309/ctl/Download/mid/26552/Default.aspx?id=65&ObjID=32229, 2022.
[54] ECHA (European Chemicals Agency), Annex XV Restriction Report - proposal for restriction of “MCCPs” (chloroalkanes with carbon chain lengths within the range from C14 to C17), Available at: https://echa.europa.eu/documents/10162/5246f2f3-926f-d339-c745-a67c1d2d289e, 2022.
[55] B. Yuan, V. Brüchert, A. Sobek, C.A. de Wit, Temporal trends of C8-C36 chlorinated paraffins in Swedish coastal sediment cores over the past 80 years, Environ. Sci. Technol. 51 (24) (2017) 14199–14208.
[56] B. Yuan, J.H. Tai, J.A. Padilla-Sánchez, E. Papadopoulou, L. Småstuen Haug, C. A. de Wit, Complex mixtures of chlorinated paraffins found in hand wipes of a Norwegian cohort, Environ. Sci. Technol. Lett. 7 (3) (2020) 198–205, https://doi.org/10.1021/acs.estlett.0c00090.
[57] T. McGrath, C. Christia, G. Poma, A. Covaci, Seasonal variation of short-, medium- and long-chain chlorinated paraffin distribution in Belgian indoor dust, Environ. Int. 170 (2022), 107616, https://doi.org/10.1016/j.envint.2022.107616.
[58] L. van Mourik, X. Wang, C. Paxman, P. Leonards, F. Wania, J. de Boer, J. Mueller, Spatial variation of short-and medium-chain chlorinated paraffins in ambient air across Australia, Environ. Pollut. 261 (2020), 114141.
[59] S. Rayne, K. Forest, Geometries of the perchlorinated and perbrominated C~ 3~ through C~ 6~ n-alkanes: a comparative density functional theory study, Nat. Preced. (2010), 1-1.
[60] M. Knobloch, F. Mathis, O. Diaz, U. Stalder, L. Bigler, S. Kern, D. Bleiner, N. Heeb, Selective and fast analysis of chlorinated paraffins in the presence of chlorinated mono-, di-, and tri-olefins with the R-based automated spectra evaluation routine (RASER), Anal. Chem. 94 (40) (2022) 13777–13784.
[61] European Commission, Council Regulation (EC) No 1881/2006 of 20/12/2006 setting Maximum levels for certain contaminants in foodstuffs, Off. J. Eur. Union L 364/5 (2006) 34–38 (Version: 01-01-2023).
[62] MEJ (Ministry of the Environment, Government of Japan), Basic Guidelines of Japan for the Promotion of Measures against Dioxins, Office of Environmental Risk Assessment, Tokyo, Japan, 1999. Available at: http://www.env.go.jp/en/chemi/dioxins/basic.pdf.
[63] US EPA (U. S. Environmental Protection Agency), Toxic Substances Control Act (TSCA), 2014. Archived from the original on October 16, 2014. Available at: https://web.archive.org/web/20141016101219/ http://www.epa.gov/agriculture/lsca.html.
[64] F. Cataldo, Synthesis of polyynes by dehydrohalogenation of chlorinated paraffins, Angew. Makromol. Chem. 264 (1) (1999) 65–72, https://doi.org/10.1002/(SICI)1522-9505(19990201)264:1<65::AID-APMC65>3.0.CO;2-9.
[65] A. Mukherjee, The Use of Chlorinated Paraffins and Their Possible Effects in the Environment. Vesi-Ja Ympäristöhallitus, 1990. P.O. Box 516, SF-00101, Helsinki, Finland. ISBN 951-47-3739-3.
[66] EFSA (European Food Safety Authority), Scientific Opinion – risk assessment of chlorinated paraffins in feed and food, EFSA J. 18 (3) (2020), e05991.
[67] L. Schinkel, C. Bogdal, E. Canonica, R. Cariou, D. Bleiner, K. McNeill, N. Heeb, Analysis of medium-chain and long-chain chlorinated paraffins: the urgent need for more specific analytical standards, Environ. Sci. Technol. Lett. 5 (12) (2018) 708–717.
[68] K. Krätschmer, A. Schächtele, R. Malisch, W. Vetter, Quantification standards-The Achilles heel of chlorinated paraffin determination, Organohalogen Compd. 81 (2019) 344–347.
[69] J. Sprengel, W. Vetter, Synthesis and characterization of eight single chain length chlorinated paraffin standards and their use for quantification, Rapid Commun. Mass Spectrom. 33 (1) (2019) 49–56.
[70] S. Valderhaug, H. Liu, A. Gorovoy, J.E. Johansen, L. van Mourik, J. de Boer, O. R. Gautun, Nuclear magnetic resonance as a tool to determine chlorine percentage of chlorinated paraffin mixtures, Chemosphere 308 (2022), 136312.
[71] M.C. Knobloch, J. Sprengel, F. Mathis, R. Haag, S. Kern, D. Bleiner, W. Vetter, N. V. Heeb, Chemical synthesis and characterization of single-chain C18-chloroparaffin materials with defined degrees of chlorination, Chemosphere 291 (P2) (2022), 132938, https://doi.org/10.1016/j.chemosphere.2021.132938.
[72] Å. Bergman, A. Rydén, R. Law, J. de Boer, A. Covaci, M. Alaee, L. Birnbaum, M. Petreas, M. Rose, N. Van den Eede, A novel abbreviation standard for organobromine, organochlorine and organophosphorus flame retardants & some characteristics of the chemicals, Environ. Int. 49 (2012) 57–82.
[73] R. Buck, J. Franklin, U. Berger, J. Conder, I. Cousins, P. De Voogt, A. Jensen, K. Kannan, S. Mabury, S. van Leeuwen, Perfluoroalkyl and polyfluoroalkyl substances in the environment: terminology, classification, and origins, Integr. Environ. Assess. Manag. 7 (4) (2011) 513–541.
[74] US EPA (U. S. Environmental Protection Agency), US EPA Chemical Data Reporting 2020 under the Toxic Substances Control Act, 2020. Available under: https://www.epa.gov/chemical-data-reporting/access-cdr-data#2020. July 2023.