ANSWERING THE URGENT CALL FOR CHLORINATED PARAFFIN STANDARDS

Chloffin

NATIVE INDIVIDUAL CONGENERS

ISO 17034
ISO/IEC 17025
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PRODUCER

What are chlorinated paraffins?

Chlorinated paraffins (CP) also known as polychlorinated n-alkanes (PCA), are produced as complex mixtures of thousands of isomers of different carbon chain length and chlorination degree.

CPs are subdivided according to their carbon chain length:

- Very short chain CPs (vSCCPs, C6–9)
- Short chain CPs (SCCPs, C10–13)
- Medium chain CPs (MCCPs, C14–17)
- Long chain CPs (LCCPs, C>17)
- Very long chain CPs (vLCCPs, >C21)

The degree of CP chlorination can vary between 30 and 70 wt%

Where are they used?

CPs are used as high-temperature lubricants in metal-working machinery and as flame retardant plasticizers in vinyl plastics. Less common applications include the use as flame retardants in textiles, rubber, paints, adhesives and as sealants.

What are the concerns?

The total global production remains largely unknown, but is believed to exceed at least two million metric tonnes per year. CPs show resistance to degradation, and some show bioaccumulation and toxic potential. They are suspected to be carcinogenic to humans according to the International Agency for Research on Cancer (IARC).

Short-chain CPs have been prohibited by the Stockholm Convention on Persistent Organic Pollutants (POPs) in the EU since 2017 (Regulation (EC)850/2004) and placed on several monitoring lists such as the EU Water Framework Directive. However, due to their persistence and long-range transport, CPs will be in the environment for decades.

Analytical challenges

One of the (many) challenges researchers face when determining CPs is the lack of suitable and generally accepted reference materials (RM). Current commercially available individual congener standards (native and labelled) have a chlorine pattern that is different than those found in industrial mixtures and the environment. CP mixture standards are not well-characterised nor purity assessed. The available labelled congener standards aimed for use as internal standard do not ionize on most commonly used detection methods (i.e. ESI and APCI). For longer chained CPs (C>17) standards in general are scarce. This all results in semi-quantitative analysis.

The CHLOFFIN project

In October 2019 the Eurostars CHLOFFIN project was launched to address the lack of suitable standards for CPs. The three year collaboration between Chiron, Vrije Universiteit and European Commission, Joint Research Centre aimed to deliver:

40 Native individual congener standards of CPs

8 ^{13}C labelled individual congener standards of CPs

10 Single chain mixtures

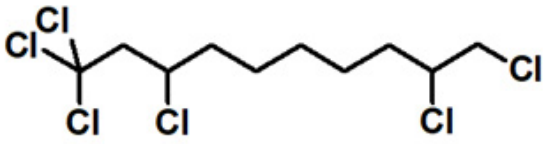
1 Matrix Certified Reference Material (CRM)

> “The lack of suitable standards for Chlorinated Paraffins has presented significant challenges for their analysis and regulation.”

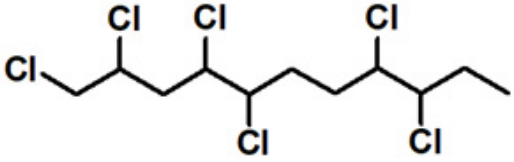
A new generation of reference materials

For ease of differentiation, Chiron have divided the available CP reference materials into three generations. The 1st generation products were developed by Chiron in the early 2000's, and some are recommended as internal standards in the ISO 12010 method for water quality determination, due to their absence in commercial products and different elution. The 2nd generation have one or two chlorines at the end of the chain and are only a minor constituent in commercial mixes. The 3rd generation products – produced through the CHLOFFIN project - are well-characterised, and purity assessed. They have similar chlorine patterns to CPs found in industrial mixtures and ionize on commonly used detection methods. These 3rd generation standards are useful in the quantification of CPs as well as helping in distinguishing the various congener groups according to carbon chain length and chlorine content. They present an important step forward in the accurate quantification of CPs and harmonization of measurement results.

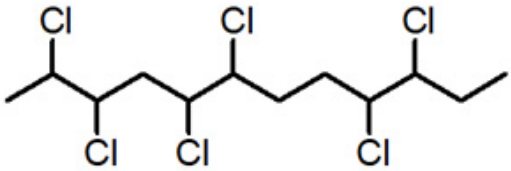
1st Generation: 3+ terminal and geminal chlorines > Not seen in commercial products



2nd Generation: 1 or 2 terminal chlorines > Minor constituent of commercial products



3rd Generation: No terminal chlorines > Major constituent of commercial products



Available reference materials

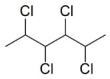
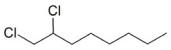
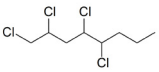
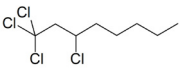
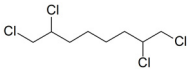
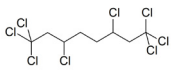
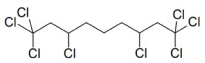
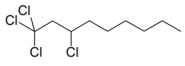
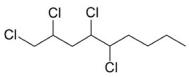
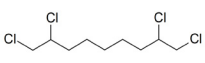
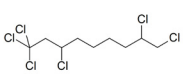
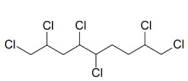
Chiron's complete range of CHLOFFIN individual congener standards are presented here.

Individual SCCPs, MCCPs and LCCPs have been prepared by chemical synthesis. The synthesis routes were designed to deliver individual CPs with defined chlorine position and number. The chemical structure is identified by NMR and MS techniques; The chemical purity is established by one or several of the following GC-based methods: GC-FID/MS, GC-MS-MS, high resolution GC-MS and GC-GC-MS.

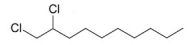
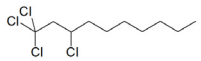
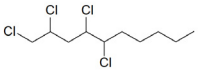
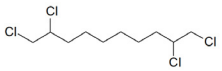
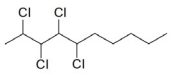
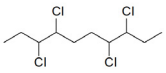
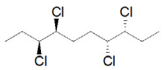
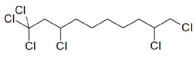
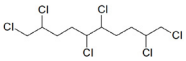
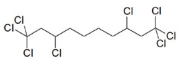
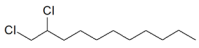
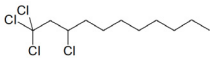
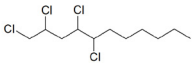
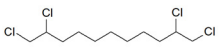
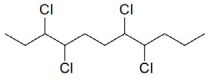
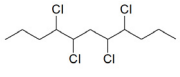
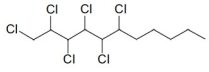
Chiron's 3rd generation reference materials will enable more accurate CP measurements and are superior to the technical mixtures, which have historically been used as reference materials.

For a quotation, please contact us today at sales@chiron.no

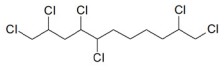
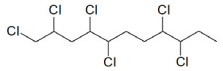
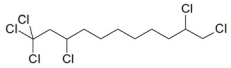
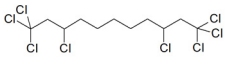
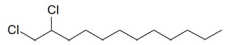
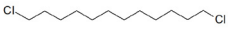
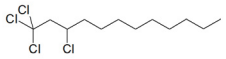
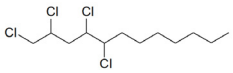
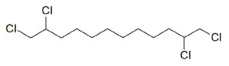
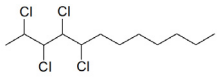
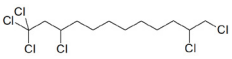
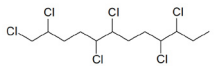
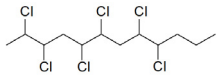
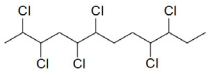
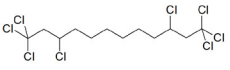
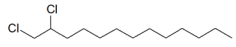
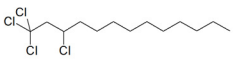
C6-C9 CPs (vSCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
3rd	CLF12287.6	2,3,4,5-Tetrachlorohexane, stereoisomers mix	63.32	$C_6H_{10}Cl_4$		N/A
2nd	CLF1664.8	1,2-Dichlorooctane	38.72	$C_8H_{16}Cl_2$		21948-46-9
2nd	CLF13254.8	1,2,4,5-Tetrachlorooctane	58.27	$C_8H_{14}Cl_4$		N/A
1st	CLF1660.8	1,1,1,3-Tetrachlorooctane	58.27	$C_8H_{14}Cl_4$		18088-13-6
2nd	CLF1672.8	1,2,7,8-Tetrachlorooctane	58.27	$C_8H_{14}Cl_4$		865306-19-0
1st	CLF1656.8	1,1,1,3,6,8,8,8-Octachlorooctane	97.87	$C_8H_{10}Cl_8$		61856-19-7
2nd	CLF1665.9	1,2-Dichlorononane	35.93	$C_9H_{18}Cl_2$		56375-96-3
1st	CLF1661.9	1,1,1,3-Tetrachlorononane	53.30	$C_9H_{16}Cl_4$		1070-27-5
2nd	CLF13396.9	1,2,4,5-Tetrachlorononane	53.30	$C_9H_{16}Cl_4$		N/A
2nd	CLF1673.9	1,2,8,9-Tetrachlorononane	53.30	$C_9H_{16}Cl_4$		865306-20-3
1st	CLF1658.9	1,1,1,3,8,9-Hexachlorononane	63.51	$C_9H_{14}Cl_6$		865306-21-4
2nd	CLF13898.9	1,2,4,5,8,9-Hexachlorononane	63.51	$C_9H_{14}Cl_6$		N/A

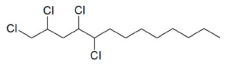
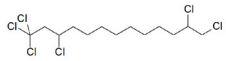
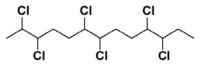
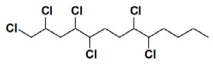
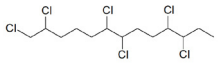
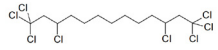
C10-C13 CPs (SCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
2nd	CLF1666.10	1,2-Dichlorodecane	33.58	$C_{10}H_{20}Cl_2$		34619-32-4
1st	CLF1662.10	1,1,1,3-Tetrachlorodecane	50.64	$C_{10}H_{18}Cl_4$		51755-60-3
2nd	CLF13255.10	1,2,4,5-Tetrachlorodecane, stereoisomers mix	50.64	$C_{10}H_{18}Cl_4$		N/A
2nd	CLF1671.10	1,2,9,10-Tetrachlorodecane	50.64	$C_{10}H_{18}Cl_4$		205646-11-3
3rd	CLF12590.10	2,3,4,5-Tetrachlorodecane, stereoisomers mix	50.64	$C_{10}H_{18}Cl_4$		N/A
3rd	CLF14965.10	3,4,7,8-Tetrachlorodecane, isomer mixture	50.64	$C_{10}H_{18}Cl_4$		N/A
3rd	CLF15252.10	(3R,4R,7S,8S)-rel-3,4,7,8-Tetrachlorodecane	50.64	$C_{10}H_{18}Cl_4$		N/A
1st	CLF1659.10	1,1,1,3,9,10-Hexachlorodecane	61.97	$C_{10}H_{16}Cl_6$		601523-26-6
2nd	CLF12284.10	1,2,5,6,9,10-Hexachlorodecane	61.97	$C_{10}H_{16}Cl_6$		189350-94-5
1st	CLF1622.10	1,1,1,3,8,10,10,10-Octachlorodecane	67.88	$C_{10}H_{14}Cl_8$		601523-23-3
2nd	CLF1667.11	1,2-Dichloroundecane	31.49	$C_{11}H_{22}Cl_2$		81246-86-8
1st	CLF1649.11	1,1,1,3-Tetrachloroundecane	48.22	$C_{11}H_{20}Cl_4$		56686-55-6
2nd	CLF13397.11	1,2,4,5-Tetrachloroundecane	48.22	$C_{11}H_{20}Cl_4$		N/A
2nd	CLF1674.11	1,2,10,11-Tetrachloroundecane	48.22	$C_{11}H_{20}Cl_4$		210049-49-3
3rd	CLF15181.11	3,4,7,8-Tetrachloroundecane, stereoisomers mix	48.22	$C_{11}H_{20}Cl_4$		N/A
3rd	CLF12728.11	4,5,7,8-Tetrachloroundecane, stereoisomers mix	48.22	$C_{11}H_{20}C_{l4}$		N/A
2nd	CLF12285.11	1,2,3,4,5,6-Hexachloroundecane, stereoisomers mix	58.60	$C_{11}H_{18}C_{l6}$		N/A

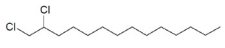
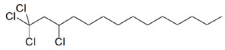
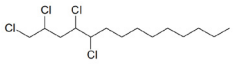
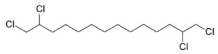
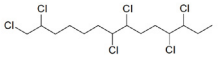
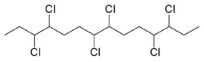
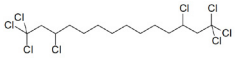
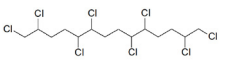
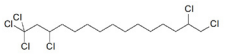
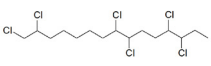
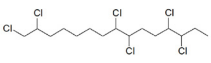
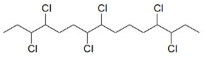
C10-C13 CPs (SCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
2nd	CLF13900.11	1,2,4,5,9,10-Hexachloroundecane, stereoisomers mix	58.60	$C_{11}H_{18}Cl_6$		N/A
2nd	CLF14069.11	1,2,4,5,8,9-Hexachloroundecane	58.60	$C_{11}H_{18}Cl_6$		N/A
1st	CLF1650.11	1,1,1,3,10,11-Hexachloroundecane	58.60	$C_{11}H_{18}Cl_6$		601523-28-8
1st	CLF1623.11	1,1,1,3,9,11,11,11-Octachloroundecane	65.67	$C_{11}H_{16}Cl_8$		601523-25-5
2nd	CLF1668.12	1,2-Dichlorododecane	29.64	$C_{12}H_{24}Cl_2$		75121-23-2
2nd	CLF1663.12	1,12-Dichlorododecane	29.64	$C_{12}H_{24}Cl_2$		3922-28-9
1st	CLF1651.12	1,1,1,3-Tetrachlorododecane	46.03	$C_{12}H_{22}Cl_4$		14983-60-9
2nd	CLF13398.12	1,2,4,5-Tetrachlorododecane	46.03	$C_{12}H_{22}Cl_4$		N/A
2nd	CLF1675.12	1,2,11,12-Tetrachlorododecane	46.03	$C_{12}H_{22}Cl_4$		210115-98-3
3rd	CLF12425.12	2,3,4,5-Tetrachlorododecane, stereoisomers mix	46.03	$C_{12}H_{22}Cl_4$		N/A
1st	CLF1652.12	1,1,1,3,11,12-Hexachlorododecane	56.42	$C_{12}H_{20}Cl_6$		865306-22-5
2nd	CLF14072.12	1,2,5,6,9,10-Hexachlorododecane	56.42	$C_{12}H_{20}Cl_6$		N/A
3rd	CLF14495.12	2,3,5,6,8,9-Hexachlorododecane	56.42	$C_{12}H_{20}Cl_6$		N/A
3rd	CLF15009.12	2,3,5,6,9,10-Hexachlorododecane; stereoisomers mix	56.42	$C_{12}H_{20}Cl_6$		N/A
1st	CLF1624.12	1,1,1,3,10,12,12,12-Octachlorododecane	63.60	$C_{12}H_{18}Cl_8$		601523-21-1
2nd	CLF1669.13	1,2-Dichlorotridecane	28.00	$C_{13}H_{26}Cl_2$		701920-72-1
1st	CLF1653.13	1,1,1,3-Tetrachlorotridecane	44.02	$C_{13}H_{24}Cl_4$		67095-50-5

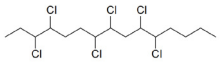
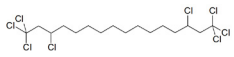
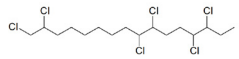
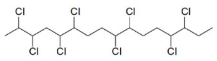
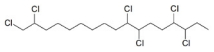
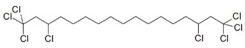
C10-C13 CPs (SCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
2nd	CLF13399.13	1,2,4,5-Tetrachlorotridecane	44.02	$C_{13}H_{24}Cl_4$		N/A
1st	CLF1654.13	1,1,1,3,12,13-Hexachlorotridecane	54.40	$C_{13}H_{22}Cl_6$		865306-23-6
3rd	CLF14496.13	2,3,6,7,10,11-Hexachlorotridecane	54.40	$C_{13}H_{22}Cl_6$		N/A
2nd	CLF15222.13	1,2,4,5,8,9-Hexachlorotridecane	54.40	$C_{13}H_{22}Cl_6$		N/A
2nd	CLF14131.13	1,2,6,7,10,11-Hexachlorotridecane	54.40	$C_{13}H_{22}Cl_6$		N/A
1st	CLF1625.13	1,1,1,3,11,13,13,13-Octachlorotridecane	61.67	$C_{13}H_{20}Cl_8$		865306-24-7

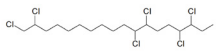
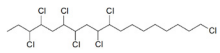
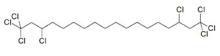
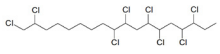
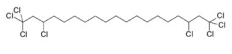
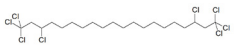
C14-C17 CPs (MCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
2nd	CLF1670.14	1,2-Dichlorotetradecane	26.53	$C_{14}H_{28}Cl_2$		701920-83-4
1st	CLF1676.14	1,1,1,3-Tetrachlorotetradecane	42.18	$C_{14}H_{26}Cl_4$		865306-25-8
2nd	CLF13256.14	1,2,4,5-Tetrachlorotetradecane	42.18	$C_{14}H_{26}Cl_4$		N/A
2nd	CLF1677.14	1,2,13,14-Tetrachlorotetradecane	42.18	$C_{14}H_{26}Cl_4$		221155-23-3
2nd	CLF14132.14	1,2,7,8,11,12-Hexachlorotetradecane	52.51	$C_{14}H_{24}Cl_6$		N/A
3rd	CLF14796.14	3,4,7,8,11,12-Hexachlorotetradecane, stereoisomer mix	52.51	$C_{14}H_{24}Cl_6$		N/A
1st	CLF1678.14	1,1,1,3,12,14,14,14-Octachlorotetradecane	59.84	$C_{14}H_{22}Cl_8$		865306-26-9
2nd	CLF14068.14	1,2,5,6,9,10,13,14-Octachlorotetradecane	59.84	$C_{14}H_{22}Cl_8$		N/A
1st	CLF8506.15	1,1,1,3,14,15-Hexachloropentadecane	50.76	$C_{15}H_{26}Cl_6$		N/A
2nd	CLF14133.15	1,2,8,9,12,13-Hexachloropentadecane, stereoisomers mix	50.76	$C_{15}H_{26}Cl_6$		N/A
2nd	CLF14475.15	1,2,8,9,12,13-Hexachloropentadecane, stereoisomers mix, cryst.	50.76	$C_{15}H_{26}Cl_6$		N/A
3rd	CLF14741.15	3,4,7,8,12,13-Hexachloropentadecane, stereoisomers mix	50.76	$C_{15}H_{26}Cl_6$		N/A

C14-C17 CPs (MCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
3rd	CLF14497.15	3,4,7,8,10,11-Hexachloropentadecane, stereoisomers mix cryst.	50.76	$C_{15}H_{26}Cl_6$		N/A
2nd	CLF13596.16	1-Chlorohexadecane	13.59	$C_{16}H_{33}Cl$		4860-03-1
1st	CLF8507.16	1,1,1,3,14,16,16,16-Octachlorohexadecane	56.50	$C_{16}H_{26}Cl_8$		N/A
2nd	CLF14134.16	1,2,9,10,13,14-Hexachlorohexadecane, stereoisomers mix	49.11	$C_{16}H_{28}Cl_6$		N/A
3rd	CLF14423.16	2,3,5,6,9,10,13,14-Octachlorohexadecane	56.50	$C_{16}H_{26}Cl_8$		N/A
2nd	CLF14135.17	1,2,10,11,14,15-Hexachloroheptadecane, stereoisomers mix	47.57	$C_{17}H_{30}Cl_6$		N/A
1st	CLF8508.17	1,1,1,3,15,17,17,17-Octachloroheptadecane	54.96	$C_{17}H_{28}Cl_8$		N/A

C18+ CPs (LCCPs):

Generation	Chiron No.	Name	%Wt Cl	Mol. Formula	Structure	CAS
2nd	CLF2051.18	1-Chlorooctadecane	12.27	$C_{18}H_{36}Cl_2$		3386-33-2
2nd	CLF14136.18	1,2,11,12,15,16-Hexachlorooctadecane, stereoisomers mix	46.12	$C_{18}H_{32}Cl_6$		N/A
3rd	CLF14071.18	3,4,6,7,9,10,18-Heptachlorooctadecane	50.07	$C_{18}H_{31}Cl_7$		N/A
1st	CLF8509.18	1,1,1,3,16,18,18,18-Octachlorooctadecane	53.51	$C_{18}H_{30}Cl_8$		N/A
2nd	CLF14070.18	1,2,9,10,12,13,15,16-Octachlorooctadecane	53.51	$C_{18}H_{30}Cl_8$		N/A
1st	CLF8510.19	1,1,1,3,17,19,19,19-Octachlorononadecane	52.13	$C_{19}H_{32}Cl_8$		N/A
1st	CLF8511.20	1,1,1,3,18,20,20,20-Octachloroeicosane	50.82	$C_{20}H_{34}Cl_8$		N/A

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