

Congener-Specific Numbering Systems for the Environmentally Relevant C₄ through C₈ Perfluorinated Homologue Groups of Alkyl Sulfonates, Carboxylates, Telomer Alcohols and Acids and Their Derivatives

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Introduction

We introduce a congener-specific numbering system for the C₄ through C₈ perfluorinated homologue groups of alkyl sulfonates, carboxylates, telomer alcohols and acids, and their derivatives. Increasing length of the carbon chain beyond C₃ leads to a corresponding rapid increase in the number of potential isomers (C₄=4, C₅=8, C₆=17, C₇=39, and C₈=89 congeners). There is a need for clear and unambiguous chemical shorthand to ensure accuracy and consistency in the future perfluorinated alkyl substance (PFA) literature, and to correct previous misconceptions that may have restricted research efforts into developing full-congener PFA analysis. If adopted by the research community, introduction of a numbering system at this relatively early stage of investigations into the congener-specific analysis, environmental behavior, and toxicology of PFAs would not require an arduous and difficult reassignment of historical structures and naming conventions presented in the prior art. Many PFA congeners are chiral (chiral centers denoted by a "*" in Figures 2 through 6), necessitating a consideration of their enantiospecific environmental behavior and toxicology.

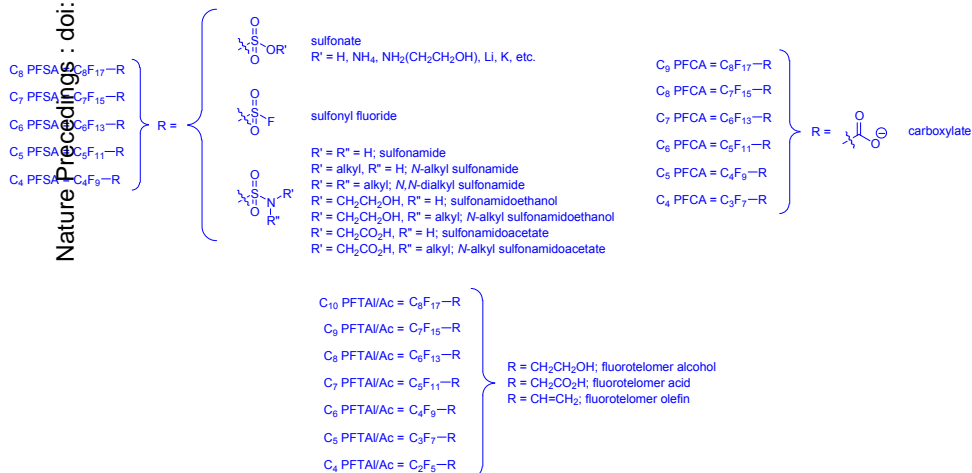


Figure 1. PFA structures for which the proposed numbering system applies.

Table 1. Number of PFA congeners and stereoisomers in each of the C₃ through C₈ homologues.

Homologue group	# of congeners	# of chiral congeners	# with 1 chiral center	# with 2 chiral centers	# with 3 chiral centers	Total number of stereoisomers
3	2	0	-	-	-	-
4	4	1	1	-	-	2
5	8	3	3	-	-	6
6	17	9	8	1	-	20
7	39	24	19	5	-	58
8	89	66	48	17	1	172

Figure 2. Structures and numbering system for the C₄ perfluorinated chains.

#	Substitution	Structure
C ₄ 1	1,1'-dimethylethyl	
2	1-methylpropyl	
3	2-methylpropyl	
4	n-butyl	

Figure 3. Structures and numbering system for the C₅ perfluorinated chains.

#	Substitution	Structure
C ₅ 1	1-ethylpropyl	
2	1,1'-dimethylpropyl	
3	1,2-dimethylpropyl	
4	2,2'-dimethylpropyl	
5	1-methylbutyl	
6	2-methylbutyl	
7	3-methylbutyl	
8	n-pentyl	

Figure 4. Structures and numbering system for the C_6 perfluorinated chains.

C_6	#	Substitution	Structure
	1	1-ethyl-1-methylpropyl	
	2	1-ethyl-2-methylpropyl	
	3	1,1',2-trimethylpropyl	
	4	1,2,2'-trimethylpropyl	
	5	1-ethylbutyl	
	6	2-ethylbutyl	
	7	1,1'-dimethylbutyl	
	8	1,2-dimethylbutyl	
	9	1,3-dimethylbutyl	
	10	2,2'-dimethylbutyl	
	11	2,3-dimethylbutyl	
	12	3,3'-dimethylbutyl	
	13	1-methylpentyl	
	14	2-methylpentyl	
	15	3-methylpentyl	
	16	4-methylpentyl	
	17	n-hexyl	

Figure 5. Structures and numbering system for the C_7 perfluorinated chains.

C_7	#	Substitution	Structure
	1	1,1'-diethylpropyl	
	2	1-ethyl-1',2'-dimethylpropyl	
	3	1-ethyl-2,2'-dimethylpropyl	
	4	2-methyl-1-isopropylpropyl	
	5	1,1',2,2'-tetramethylpropyl	
	6	1-ethyl-1'-methylbutyl	
	7	1-ethyl-2-methylbutyl	
	8	1-ethyl-3-methylbutyl	
	9	2-ethyl-1-methylbutyl	
	10	2-ethyl-2'-methylbutyl	
	11	2-ethyl-3-methylbutyl	
	12	1,1',2-trimethylbutyl	
	13	1,1',3-trimethylbutyl	
	14	1,2,2'-trimethylbutyl	
	15	1,2,3-trimethylbutyl	
	16	1,3,3'-trimethylbutyl	
	17	2,2',3-trimethylbutyl	
	18	2,3,3'-trimethylbutyl	
	19	1-isopropylbutyl	
	20	1-propylbutyl	
	21	1-ethylpentyl	
	22	2-ethylpentyl	
	23	3-ethylpentyl	
	24	1,1'-dimethylpentyl	
	25	1,2-dimethylpentyl	
	26	1,3-dimethylpentyl	
	27	1,4-dimethylpentyl	
	28	2,2'-dimethylpentyl	
	29	2,3-dimethylpentyl	
	30	2,4-dimethylpentyl	
	31	3,3'-dimethylpentyl	
	32	3,4-dimethylpentyl	
	33	4,4'-dimethylpentyl	
	34	1-methylhexyl	
	35	2-methylhexyl	
	36	3-methylhexyl	
	37	4-methylhexyl	
	38	5-methylhexyl	
	39	n-heptyl	

#	Substitution	Structure	#	Substitution	Structure	#	Substitution	Structure	#	Substitution	Structure
1	1-ethyl-1',2,2'-trimethylpropyl		22	2-ethyl-3,3'-dimethylbutyl		43	3-ethyl-3'-methylpentyl		64	1-ethylhexyl	
2	1-ethyl-1'-isopropylpropyl		23	1,1',2,2'-tetramethylbutyl		44	3-ethyl-4-methylpentyl		65	2-ethylhexyl	
3	1-isopropyl-1',2-dimethylpropyl		24	1,1',2,3-tetramethylbutyl		45	1-isopropylpentyl		66	3-ethylhexyl	
4	1-isopropyl-2,2'-dimethylpropyl		25	1,1',3,3'-tetramethylbutyl		46	2-isopropylpentyl		67	4-ethylhexyl	
5	1-tert-butyl-butyl		26	1,2,2',3-tetramethylbutyl		47	1,1',2-trimethylpentyl		68	1,1'-dimethylhexyl	
6	1,1'-diethylbutyl		27	1,2,3,3'-tetramethylbutyl		48	1,1',3-trimethylpentyl		69	1,2-dimethylhexyl	
7	1,2-diethylbutyl		28	2,2',3,3'-tetramethylbutyl		49	1,1',4-trimethylpentyl		70	1,3-dimethylhexyl	
8	2,2'-diethylbutyl		29	2,2',4,4'-tetramethylbutyl		50	1,2,2'-trimethylpentyl		71	1,4-dimethylhexyl	
9	1-isopropyl-1'-methyl-butyl		30	1-propyl-1'-methylbutyl		51	1,2,3-trimethylpentyl		72	1,5-dimethylhexyl	
10	1-isopropyl-2-methylbutyl		31	1-propyl-2-methylbutyl		52	1,2,4-trimethylpentyl		73	2,2'-dimethylhexyl	
11	1-isopropyl-3-methylbutyl		32	1-propyl-3-methylbutyl		53	1,3,3'-trimethylpentyl		74	2,3-dimethylhexyl	
12	2-isopropyl-3-methylbutyl		33	1-ethyl-1'-methylpentyl		54	1,3,4-trimethylpentyl		75	2,4-dimethylhexyl	
13	1-ethyl-1',2-dimethylbutyl		34	1-ethyl-2-methylpentyl		55	1,4,4'-trimethylpentyl		76	2,5-dimethylhexyl	
14	1-ethyl-1,3-dimethylbutyl		35	1-ethyl-3-methylpentyl		56	2,2',3-trimethylpentyl		77	3,3'-dimethylhexyl	
15	1-ethyl-2,2'-dimethylbutyl		36	1-ethyl-4-methylpentyl		57	2,3,3'-trimethylpentyl		78	3,4-dimethylhexyl	
16	1-ethyl-2,3-dimethylbutyl		37	2-ethyl-1-methylpentyl		58	2,3,4-trimethylpentyl		79	3,5-dimethylhexyl	
17	1-ethyl-3,3'-dimethylbutyl		38	2-ethyl-2-methylpentyl		59	2,4,4'-trimethylpentyl		80	4,4'-dimethylhexyl	
18	2-ethyl-1,1'-dimethylbutyl		39	2-ethyl-3-methylpentyl		60	3,3',4-trimethylpentyl		81	4,5-dimethylhexyl	
19	2-ethyl-1,2'-dimethylbutyl		40	2-ethyl-4-methylpentyl		61	3,4,4'-trimethylpentyl		82	5,5'-dimethylhexyl	
20	2-ethyl-1,3-dimethylbutyl		41	3-ethyl-1-methylpentyl		62	1-propylpentyl		83	1-methylheptyl	
21	2-ethyl-2',3-dimethylbutyl		42	3-ethyl-2-methylpentyl		63	2-propylpentyl		84	2-methylheptyl	

85	3-methylheptyl	
86	4-methylheptyl	
87	5-methylheptyl	
88	6-methylheptyl	
89	n-octyl	

Figure 6. Structures and numbering system for the C₈ perfluorinated chains.

Conclusion

The proposed numbering system for PFAs presented herein offers a concise and unambiguous means for communicating molecular structures of these important contaminants within the scientific literature. In addition, the system outlines the number and range of possible structures that may be present in environmental and biological systems, and for which more comprehensive congener-specific analysis and testing methods should be developed.

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