Re-evaluating the list of high-production chemicals predicted to become Arctic contaminants

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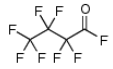
The large number of historical and current organic chemicals in commerce, and the ability of these compounds to make their way from industrial to remote regions, has resulted in concerted efforts to predict which chemicals have the capacity to migrate from where they are used/disposed to areas such as the Arctic.[1-5] In the absence of reliable experimental data on the physicochemical properties of most commercial chemicals, and the lack of resources for monitoring environmental samples for all possible analytes, substantial progress has been made using computational tools such as property estimation programs (e.g., EPI Suite, COSMOtherm, SPARC, etc.) in concert with multimedia models (e.g., CalTOX, CEMCLIII, SimpleBOX, ChemRange, ELPOS, Globo-POP, BETR, etc.) to assess whether current or legacy compounds may be contaminating remote regions.[6,7] These methods are also used to predict which new compounds and structural functionalities are likely to be sufficiently persistent, bioaccumulative, toxic, and amenable to long range transport to pose a risk to Arctic ecosystems. In recent work, a suite of 120 high production volume chemicals were screened from an initial dataset of >100,000 compounds as potential Arctic contaminants.[8] In the current work, we critically assess members of this proposed list for their possible rapid reactivity in environmental systems that would prevent substantial accumulation or transport in the environment and accumulation in vivo, as well as whether the investigated physicochemical properties are adequate for the intended environmental screening purposes.

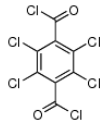
The list of 120 proposed potential Arctic contaminants is given in Appendix Table 1. The following five acyl halides are present in the list:



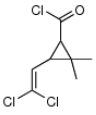
heptafluorobutanoyl fluoride
(CAS 335422)

1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonyl fluoride
(CAS 423507)

perfluoro-1-octanesulfonyl fluoride
(CAS 307357)



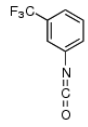
2,3,5,6-tetrachloro-1,4-benzenedicarbonyl dichloride
(CAS 719324)



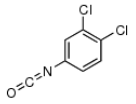
3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarbonyl chloride
(CAS 52314677)

Acyl halides are too reactive toward aqueous or atmospheric hydrolysis to be transported intact from industrial sources to remote regions, or to exist long in environmental systems or in vivo. Rapid hydrolysis of these compounds would form the corresponding acids (perfluorobutanoic acid in the case of CAS 335422, the perfluorohexane and perfluorooctane sulfonic acids for CAS 423507 and 307357, respectively, and the carboxylic acids for CAS 719324 and 52314677). A threshold persistence from several months to a year in surface media has been postulated as a prerequisite for the possibility of significant Arctic contamination.[2] Hydrolysis rates of acyl halides in various environmental media, including surface waters, soils, the atmosphere, and in vivo, will be much shorter than these thresholds. Thus, acyl halides should not likely be present on a list of potential candidates that requires compounds to be sufficiently persistent to become Arctic contaminants.

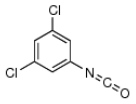
Similarly, isocyanates (e.g., CAS 329011, 102363, and 34893920), epoxides (e.g., 428591), anhydrides (e.g., 115275), and peroxides (e.g., 78637 and 3457612) are also reactive toward hydrolysis. This suggests the following compounds (and similar molecules) should perhaps also be removed from potential Arctic contaminant screening lists due to their likely very short persistence in environmental and biological systems:



1-isocyanato-3-(trifluoromethyl)benzene
(CAS 329011)

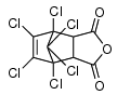


1,2-dichloro-4-isocyanatobenzene
(CAS 102363)

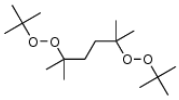


1,3-dichloro-5-isocyanatobenzene
(CAS 34893920)

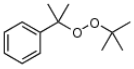
trifluoro(trifluoromethyl)oxirane
(CAS 428591)



chlorendic anhydride
(CAS 115275)



(1,1,4,4-tetramethyl-1,4-butanediyl)bis(1,1-dimethylethyl)peroxide
(CAS 786637)



1,1-dimethylethyl 1-methyl-1-phenylethylperoxide
(CAS 3457612)

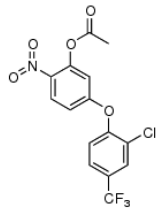
The reactivity of alkyl halides varies substantially depending on the halide under consideration, the electron withdrawing or releasing nature of substituents on the alkyl chain, as well as any steric hindrance in the molecule. We have previously shown that fluorotelomer iodides may have hydrolytic half-lives of ~130 days in natural waters,[9] suggesting that CAS 2043530 and 2043541 may not be sufficiently persistent to become potential Arctic contaminants.

1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iododecane
(CAS 2043530)

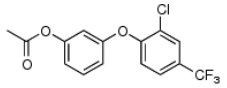
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoro-12-iododododecane
(CAS 2043541)

Several carboxylic acid esters have also been proposed as possible Arctic contaminants. As with the other classes considered above, the carboxylic acid esters are susceptible to abiotic hydrolysis. Using the SPARC

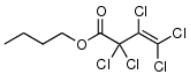
hydrolysis module (September 2009 release w4.5.1529-s4.5.1529; http://ibmlc2.chem.uga.edu/sparc/), which we [9] and others [10] have validated, we estimate the following half-lives for these esters: CAS 50594440, 4 hours; CAS 50594779, 22 days; CAS 75147205, 5 min; CAS 60825265, 63 days; and CAS 1539044, 215 days.



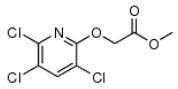
phenol, 5- 2-chloro-4-(trifluoromethyl)phenoxy -2-nitro-, acetate
(CAS 50594440)



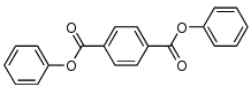
phenol, 3- 2-chloro-4-(trifluoromethyl)phenoxy -, acetate
(CAS 50594779)



3-butenoic acid, 2,2,3,4,4-pentachloro-, butyl ester
(CAS 75147205)



(3,5,6-trichloro-2-pyridinyl)oxy-acetic acid, methyl ester
(CAS 60825265)

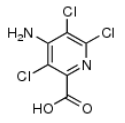


diphenyl terephthalate
(CAS 1539044)

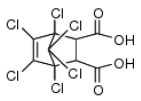
With short half-lives, these esters are not persistent. Depending on their current use and atmospheric transport patterns, under a strong kinetic flux from industrialized regions, Arctic accumulation could occur (similar to α- and β-endosulfan, which have hydrolytic half lives of 11 and 19 days, respectively,[11] but which are known to occur widely in Arctic regions [12,13] due to continuing fluxes that offset in situ degradation rates).

The cobalt(2+) salt of neodecanoic acid (CAS 52270447; a mixture of branched alkylcarboxylic acids with the common structural formula $C_{10}H_{20}O_2$) has been proposed as a potential Arctic contaminant. Transition metal (TM) carboxylate salts would be relatively non-volatile, and any aquatic exposure between industrialized and remote regions would result in cation exchange, leading to a dominantly non-TM counterion such as Na^+, Ca^{2+}, etc. Any consideration of neodecanoic acid as an environmental contaminant should likely be as either its neutral form (proton countercation) or strictly as the carboxylate form.

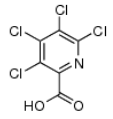
Finally, several acidic compounds have been proposed as Arctic contaminants (e.g., CAS 1918021, 115286, 10469097, 335671, 88062, 118796, 88857, 98737, 320729, 63734623, and 133493). In general, molecular (undissociated) forms of chemicals are substantially more volatile than the anionic (dissociated) forms. Thus, in K_{ow}/K_{aw} (octanol-water partitioning coefficient/air-water partitioning coefficient) based screening assessments for modes and potential of Arctic contamination (e.g. ref. [1-8]), the anionic forms (even for weak acids) need to be explicitly taken into account. A similar requirement applies for weak and strong bases being considered for Arctic contamination potential and other environmental fate modeling. Most K_{ow}/K_{aw} calculations conducted on these acids only consider the molecular form, although in the majority of cases the acids are sufficiently strong that the molecules are effectively completely dissociated under most environmental and biological conditions.



picloram
(CAS 1918021)

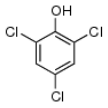


1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid
(CAS 115286)

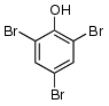


3,4,5,6-tetrachloro-2-pyridinecarboxylic acid
(CAS 10469097)

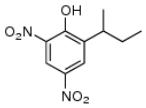
pentadecafluorooctanoic acid
(CAS 335671)



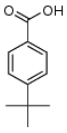
2,4,6-trichlorophenol
(CAS 88062)



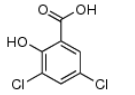
2,4,6-tribromophenol
(CAS 118796)



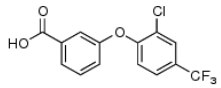
dinoseb
(CAS 88857)



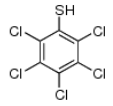
p-tert-butylbenzoic acid
(CAS 98737)



3,5-dichloro-2-hydroxybenzoic acid
(CAS 320729)



3-(2-chloro-4-trifluoromethylphenoxy)-benzoic acid
(CAS 63734623)



pentachlorobenzenethiol
(CAS 133493)

For example, the pK_a of pentachlorobenzenethiol (CAS 133493) is predicted by the SPARC acidity constant estimation module (September 2009 release w4.5.1529-s4.5.1529; http://ibmlc2.chem.uga.edu/sparc/) to be 1.91, or a modestly strong acid. 2,4,6-Trichlorophenol (CAS 88062) and 2,4,6-tribromophenol (CAS 118796) have experimental pK_a values of 6.00 [14,15] and 6.08,[16] respectively. n-PFOA (CAS 335671) has an experimental pK_a of ~0 [17] in excellent agreement with computational

estimates.[18-20] For the five remaining acids, SPARC estimated pK_a values are 2.66 (CAS 1918021), 1.46 (CAS 115286), 2.15 (CAS 10469097), 5.52 (CAS 88857), 5.20 (CAS 98737), 2.22 (CAS 320729), and 3.64 (CAS 63734623).

The substantial, if not effectively complete, dissociation of these acids in aqueous solution will significantly affect their physicochemical properties. In Figure 1, we present the SPARC estimated log D_{ow} (octanol-water distribution coefficient) and log K_{aw} as functions of pH for these 11 acidic compounds on the potential Arctic contaminant screening list.

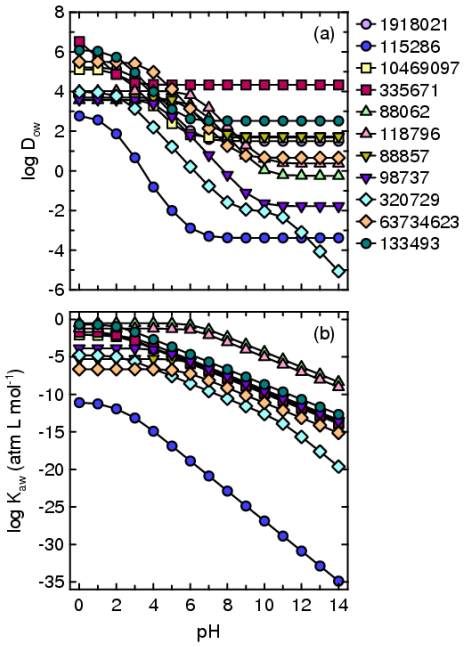


Figure 1. SPARC estimated log D_{ow} and log K_{aw} as a function of pH for 11 acidic compounds on the potential Arctic contaminant screening list.

As expected, the log D_{ow} and log K_{aw} both decline substantially with increasing pH, as the molecules deprotonate to the less lipophilic and less volatile anionic forms. Differences of up to 9 log D_{ow} units are observed between the molecular and fully deprotonated forms of some compounds, and differences of up to 6 log D_{ow} units are found between the molecular species and the composite speciation present at pH 7. In a number of cases, the molecular form is predicted to be substantially lipophilic, whereas the anionic form is predicted to be substantially hydrophilic. The effect of ionization has a greater pH dependent influence on the K_{aw}. Differences of up to 24 log K_{aw} units occur between the molecular and fully deprotonated forms, and up to 10 log K_{aw} units between the molecular species and the composite speciation at pH 7.

Consequently, in any K_{ow}/K_{aw} based screening assessment for Arctic contamination potential, the acidity/basicity of all compounds at relevant pH values (varying depending on nature of the freshwater, marine, soil, atmospheric, or biological system under study) must explicitly be taken into consideration. Otherwise, spurious and/or erroneous long range transport potential and bioaccumulation potential conclusions are likely. Within this context, current lists of potential Arctic contaminants likely require additional screening and modeling efforts that more fully incorporate knowledge regarding likely rapid reactivity in environmental systems, and using physicochemical properties more relevant to the systems under investigation.

References and Notes

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Appendix Table 1. List high production volume chemicals predicted to become Arctic contaminants or which match the structural profile of known Arctic contaminants. Taken from ref. [8].

CAS	Name
115286	1,4,5,6,7,7-hexachloro-5-norbornene-2,3-dicarboxylic acid
1691992	N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-1-octanesulfonamide
2157199	endosulfan alcohol
25637994	hexabromocyclododecane (1,3,5,7,9,11-hexabromocyclododecane)
27905459	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl, 2-propenoic acid ester
61262531	1,1′-[1,2-ethanediylbis(oxy)]bis-2,3,4,5,6-pentabromobenzene
77474	1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene
87616	1,2,3-trichlorobenzene
87683	1,1,2,3,4,4-hexachloro-1,3-butadiene
98157	1-chloro-3-(trifluoromethyl)-benzene
98464	1-nitro-3-(trifluoromethyl)-benzene
98566	1-chloro-4-(trifluoromethyl)-benzene
108770	2,4,6-trichloro-1,3,5-triazine
115253	octafluorocyclobutane
120821	1,2,4-trichlorobenzene
307357	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-1-octanesulfonyl fluoride
311897	1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(nonafluorobutyl)-1-butanamine
328847	1,2-dichloro-4-(trifluoromethyl)-benzene
329011	1-isocyanato-3-(trifluoromethyl)-benzene
335422	heptafluoro-butanoyl fluoride
338841	1,1,2,2,3,3,4,4,5,5,5-undecafluoro-N,N-bis(undecafluoropentyl)-pentanamine
423507	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonyl fluoride
428591	trifluoro(trifluoromethyl)-oxirane
647427	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-octanol
678397	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decanol
719324	2,3,5,6-tetrachloro-1,4-benzenedicarbonyl dichloride
865861	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluoro-1-dodecanol
1163195	decabromodiphenylether
1737935	3,5-dichloro-2,4,6-trifluoropyridine
1897456	chlorothalonil
1918021	picloram
1929824	nitrapyrin
2043530	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iododecane
2043541	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoro-12-iodododecane
2043574	1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane
2402791	2,3,5,6-tetrachloropyridine
3194556	1,2,5,6,9,10-hexabromocyclododecane
3825261	ammonium perfluorooctanoate
5848931	5-chloro-3-(trichloromethyl)-1,2,4-thiadiazole
10469097	3,4,5,6-tetrachloro-2-pyridinecarboxylic acid
14143603	4-amino-3,5,6-trichloro-2-pyridinecarbonitrile
17824838	3,4,5,6-tetrachloro-2-pyridinecarbonitrile
32534819	pentabromodiphenylether (BDE-99)
32536520	octabromodiphenylether (BDE-203)
36483600	hexabromodiphenylether (BDE-167)
40088479	tetrabromodiphenylether (BDE-55)
52314677	3-(2,2-dichloroethenyl)-2,2-dimethyl-cyclopropanecarbonyl chloride
59808785	tetrachlorocyclopentane (1,2,3,4-tetrachlorocyclopentane)
60825265	(3,5,6-trichloro-2-pyridinyl)oxy-acetic acid, methyl ester
63936561	nonabromodiphenylether (BDE-206)
68928803	heptabromodiphenylether (BDE-173)
69045789	2-chloro-5-trichloromethylpyridine
86508421	perfluoro compounds $C_{5\text{-}18}$ (perfluoroundecane)
138495428	1,1,1,2,2,3,4,5,5,5-decafluoropentane
163702076	1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-butane
101053	anilazine
115275	1,4,5,6,7,7-hexachloro-5-norbornene-2,3-dicarboxylic anhydride
115297	endosulfan
3278895	1,3,5-tribromo-2-(2-propenyloxy)-benzene
3734483	chlordene
24448097	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-N-methyl-1-octanesulfonamide
78637	1,1′-(1,1,4,4-tetramethyl-1,4-butanediyl)bis[2-(1,1-dimethylethyl) peroxide
80079	1,1′-sulfonylbis[4-chlorobenzene]
80104	dichlorodiphenylsilane
81141	1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]-ethanone
81152	1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitrobenzene
84515	2-ethyl-9,10-anthracenedione
88062	2,4,6-trichlorophenol
88857	dinoseb
98737	4-(1,1-dimethylethyl)-benzoic acid
101633	1,1′-oxybis 4-nitrobenzene

102363	1,2-dichloro-4-isocyanatobenzene
115322	dicofol
118796	2,4,6-tribromophenol
136607	benzoic acid, butyl ester
144796	chloromethyldiphenylsilane
147820	2,4,6-tribromobenzenamine
320729	3,5-dichloro-2-hydroxybenzoic acid
540976	2,2,4,4,6,6,8,8,10,10,12,12-dodecamethylcyclohexasiloxane
1185097	1,1,2,2-tetrachloro-ethanesulfenyl chloride
1539044	1,4-benzenedicarboxylic acid, 1,4-diphenyl ester
1836755	nitrofen
2116849	1,1,1,5,5,5-hexamethyl-3-phenyl-3-[(trimethylsilyl)oxy]-trisiloxane
2392485	4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene
3457612	1,1-dimethylethyl 1,1-dimethylethyl peroxide
13472087	2,2′-azobis-2-methylbutanenitrile
34893920	1,3-dichloro-5-isocyanatobenzene
35578473	bis(4-bromophenyl)-ethanedione
50594440	5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrophenol, 1-acetate
50594779	3-[2-chloro-4-(trifluoromethyl)phenoxy]-phenol, 1-acetate
52270447	neodecanoic acid, cobalt(2+) salt
63734623	3-(2-chloro-4-trifluoromethylphenoxy)-benzoic acid
64667330	4,6,6,6-tetrachloro-3,3-dimethylhexanoic acid methyl ester
50293	p,p′-DDT
58899	γ-HCH
68360	1,4-bis(trichloromethyl)-benzene
82688	pentachloronitrobenzene
87843	1,2,3,4,5-pentabromo-6-chlorocyclohexane
95943	1,2,4,5-tetrachlorobenzene
117088	4,5,6,7-tetrachloro-1,3-isobenzofurandione
118741	HCB
133493	pentachlorobenzenethiol
626391	1,3,5-tribromobenzene
632791	4,5,6,7-tetrabromo-1,3-isobenzofurandione
634662	1,2,3,4-tetrachlorobenzene
1134049	2,3,4,5-tetrachloro-6-(trichloromethyl)-pyridine
1203867	2,2-dichloro-1-(2,4,5-trichlorophenyl)-ethanone
1817136	3,6-dichloro-2-(trichloromethyl)-pyridine
2176627	pentachloropyridine
5216251	1-chloro-4-(trichloromethyl)-benzene
17700093	2,3,4-trichloronitrobenzene
29091096	2,4-dichloro-1,3-dinitro-5-(trifluoromethyl)-benzene
30554724	tetrabromodichlorocyclohexane (1,2,3,4-tetrabromo-5,6-dichlorocyclohexane)
62111471	heptachlorocyclopentene (1,2,3,3,4,4,5-heptachloro-1-cyclopentene)
68258902	heptachlorocyclopentane (1,2,3,3,4,5,5-heptachlorocyclopentane)
68258913	hexachlorocyclopentane (1,2,2,3,4,4-hexachlorocyclopentane)
69045836	2,3-dichloro-5-trichloromethylpyridine
72030263	hexachlorocyclopentene (1,2,3,4,5,5-hexachloro-1-cyclopentene)
73588428	1,3-dichloro-5-(1,3,3,3-tetrachloro-1-methylpropyl)-benzene
75147205	2,2,3,4,4-pentachloro-3-butenoic acid, butyl ester