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## IDENTIFICATION OF TRACE ORGANIC CONTAMINANTS IN INORGANIC WATER TREATMENT CHEMICALS BY GAS CHROMATOGRAPHY–MASS SPECTROMETRY

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### SUMMARY

Methodology is developed for the isolation and identification of organic constituents present in inorganic water treatment chemicals. Solid and liquid samples are analyzed by gas chromatography–mass spectrometry using two complementary ionization techniques, electron impact and positive ion chemical ionization. Actual samples representative of the most commonly employed water treatment chemicals were obtained from a variety of sources. The majority of the organic contaminants found to be present in these samples contain only carbon, hydrogen, oxygen, and in some cases nitrogen. In the twenty-four samples analyzed only a total of three chlorinated species were identified. The total organic content of the various chemicals studied was found to range from 0.01 to 300 ppm, however, most samples contained less than 10 ppm.

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### INTRODUCTION

Testing of the quality of drinking water is performed on a routine basis in many North American cities. The majority of the research carried out is devoted to the development and improvement of methods for the determination of either organic or inorganic species in the final product of the water purification process<sup>1–8</sup>. However, it is also important that the sources of contaminants be recognized so that measures can be taken to reduce the presence of these materials. This study is concerned with the development of methodology for the isolation and identification of trace organic contaminants present in the inorganic chemicals typically employed in the water treatment process. This methodology is then used to analyze a series of chemicals actually utilized for water treatment.

The use of gas chromatographic–mass spectrometric (GC–MS) techniques has proven to be very useful in the analysis of complex organic mixtures. The mass spectrometer is an ideal detector for the gas chromatograph because of its sensitivity and specificity. Unlike detectors more commonly used, such as flame ionization and electron-capture detectors, the mass spectrometer can supply a tremendous amount of information regarding the structure of each individual analyte. Thus in a single

GC-MS analysis it is possible to obtain information about the structure and retention time behaviour of a particular component.

Compound identifications in this study are based mainly on the comparison of the electron impact (EI) mass spectrum of the unknown component with the spectra of a large number of reference compounds. This process is carried out by the computer data system using the Probability Based Matching (PBM) algorithm<sup>9</sup>. However, because there are many cases where compounds give very nearly identical EI mass spectra, identifications based on this information were supplemented with data from a second ionization technique, positive ion chemical ionization (PICI), a "soft" ionization technique in which relatively little fragmentation is observed using methane as the reagent gas<sup>10</sup>. Therefore it is often possible to obtain molecular weight information which may have been lacking or inconclusive based on the corresponding EI mass spectrum. By combining the complementary information obtained from the EI and PICI techniques with retention time data for any available standards, which can often be used to differentiate between isomers, positive compound identifications can be made.

The analytical methodology developed and used in this study for the analysis

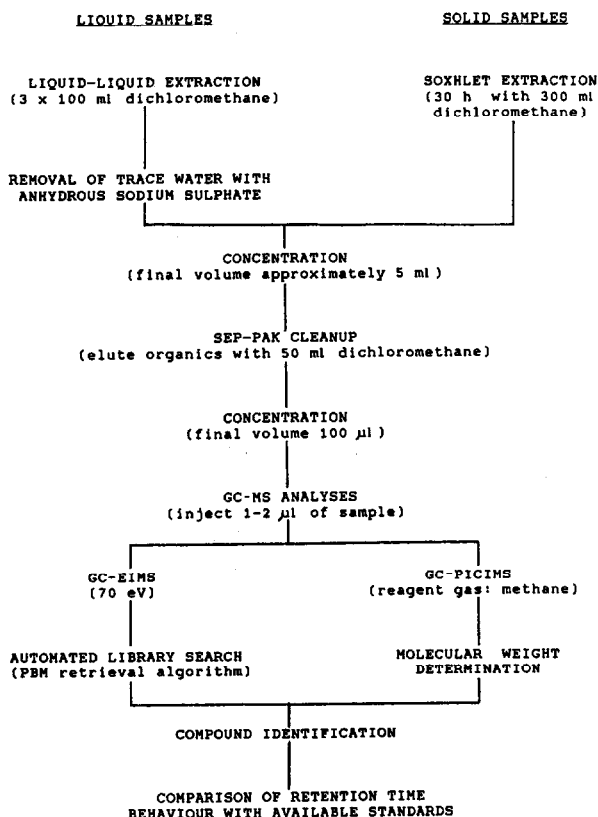


Fig. 1. Analytical scheme for the isolation and identification of trace organic contaminants in water treatment chemicals.

of trace organic contaminants in water treatment chemicals is outlined in the diagram shown in Fig. 1.

## EXPERIMENTAL

### *Chemicals*

The solvents used in this study were dichloromethane and methanol (distilled-in-glass; Caledon Labs., Georgetown, Canada). Anhydrous sodium sulphate (reagent grade; J. T. Baker, Phillipsburg, NJ, U.S.A.) was purified by means of sequential Soxhlet extraction with methanol followed by dichloromethane. The purified sodium sulphate was then stored in a stoppered glass flask and kept in an oven heated to 200°C.

The methane used as the reagent gas in the chemical ionization studies was ultrahigh purity grade (Union Carbide Canada, Toronto, Canada).

Standard solutions used for obtaining retention time data as well as mass spectra for the user-created data base were made up using standards available from PolyScience (Chemical Division, Niles, IL, U.S.A.) and from a variety of other commercial sources.

### *Glassware cleaning*

In the analysis of trace organic compounds, special precautions must be taken to ensure that contamination of the sample does not occur during the sample preparation procedure. It is therefore necessary to clean glassware which comes in contact with the sample to be analyzed. The glassware used in this study was washed in an ultrasonic bath with a mild detergent for approximately 30 min. Individual pieces are then rinsed with large quantities of deionized water and dried overnight in an oven at 275°C. All glassware is rinsed three times with dichloromethane immediately before use. Soxhlet extraction apparatus is rinsed by setting the equipment up in the normal fashion and extracting the empty apparatus with 300 ml of dichloromethane for 2 h.

### *Sample preparation*

All solid samples were extracted for 30 h with 300 ml of dichloromethane using Soxhlet extraction apparatus. Each sample was extracted in duplicate and a blank was also run using a complete but empty extraction apparatus. The amount of solid extracted was set by the volume limitations of the extraction thimbles used and was found to be approximately 100 ml for efficient extraction. After the extraction period had elapsed, the resulting organic mixture was then concentrated down to approximately 1 ml using rotary evaporation. The extract was then transferred, rinsing the collection flask with dichloromethane, to a small glass vial such that the total volume of the extract and rinsings was about 5 ml.

A 500-ml volume of liquid sample is extracted with three 100-ml aliquots of dichloromethane using a 1-l separatory funnel. The combined extract is then passed through a sintered glass crucible containing approximately 20 g of purified sodium sulphate in order to remove traces of water which may be present. The sodium sulphate is then rinsed with 50 ml of fresh dichloromethane once the entire sample extract has been passed through it. The resulting organic mixture is then concentrated and transferred to a small glass vial giving a final volume of approximately 5 ml.

Unlike the other liquid samples which were analyzed, hydrofluorosilicic acid can be particularly hazardous to work with because it shows many of the same chemical properties as hydrofluoric acid. Its corrosiveness towards glassware requires that polypropylene separatory funnels be used in place of the conventional glass apparatus. The hydrofluorosilicic acid samples are otherwise extracted using the same procedure employed for the other liquid samples.

Some of the inorganic salts found in the water treatment chemicals show a limited solubility in dichloromethane. This can cause considerable problems in the chromatographic analyses as these salts are retained on the column due to their high boiling points and here they act as active sites. These active sites result in the broadening of peak shapes for compounds which are even slightly polar in nature. As a result of this, a cleanup procedure to remove them is necessary prior to analysis by GC-MS.

Each concentrated extract is passed through a Sep-Pak silica cartridge (Millipore, Waters Assoc., Milford, MA, U.S.A.) which has been pre-wet with 10 ml of dichloromethane. This is accomplished using a 50 ml gas-tight syringe with a Luer end fitting. The inorganic salts are irreversibly adsorbed on the polar stationary phase while the organics are eluted by passing 50 ml of dichloromethane through the cartridge. The eluate is collected and concentrated down to about 1 ml using rotary evaporation. The extract is then transferred to a precalibrated vial and concentrated down to a final volume of 100  $\mu$ l using a gentle stream of high purity nitrogen gas (Union Carbide).

### *Instrumentation*

All analyses were carried out using a Hewlett-Packard HP5987A gas chromatograph-mass spectrometer equipped with an HP1000 data system and an HP7914 Winchester disk drive. An HP5880A gas chromatograph is linked to the quadrupole mass spectrometer by a direct capillary inlet interface such that all of the column effluent enters the ion source. Chromatographic separations were obtained using a 30 m  $\times$  0.25 mm I.D. Supelcowax 10 fused-silica capillary column (Supelco Canada, Oakville, Canada) which had a film thickness of 0.25  $\mu$ m. Helium was used as the carrier gas with a flow-rate of 1.1 ml/min. A cool on-column injector was employed in all chromatographic analyses in order to minimize discrimination against both low and high boiling point compounds. The GC oven temperature program used was as follows: initial temperature 45°C ramped at 3°C/min to a final temperature of 270°C which was then held for 15 min.

The HP5987A GC-MS system has capabilities for several different ionization modes including EI, PICI, and negative ion chemical ionization (NICI). In EI operation the mass spectrometer is tuned using an automatic tuning program known as AUTOTUNE which is provided by Hewlett-Packard. This program adjusts the mass spectrometric parameters to meet the predetermined performance criteria using the reference compound perfluorotributylamine (PFTBA). In PICI, however, the mass spectrometer must be manually tuned using the reference compounds benzophenone and PFTBA. The various mass spectrometric parameters are optimized while monitoring the  $[M + H]^+$  ion ( $m/z$  183) of benzophenone. The mass axis is then calibrated using  $m/z$  183 from benzophenone and two ions from methane PICI mass spectrum of PFTBA,  $m/z$  414 and 652.

TABLE I  
EI AND PICI MASS SPECTROMETRIC CONDITIONS

A/D = Analog-to-digital.

Parameter	Ionization mode	
	EI	PICI
Source pressure (Torr)	$3 \cdot 10^{-6}$	1.6
Source temperature (°C)	200	200
Interface oven temperature (°C)	270	270
Scan range (a.m.u.)	50-500	60-500
Scan cycle time (ms)	0.92	0.78
Scan increment size (a.m.u.)	0.125	0.125
Scan start time (min)	2.80	2.80
A/D samples	4	4
Emission current ( $\mu$ A)	300	300
Electron energy (eV)	70	255
Electron multiplier voltage (V)	2200	2200

The mass spectrometric parameters for both ionization techniques are summarized in Table I.

The GC-MS data system employed in this study utilizes two different mass spectral data bases in its computerized search program. The data base available from the instrument supplier is made up from the NIH/EPA/MSDC Mass Spectral Data Base (NBS Library) and the Registry of Mass Spectral Data (Wiley Library). This data base contains 76 862 mass spectra, some of which are the same compound run

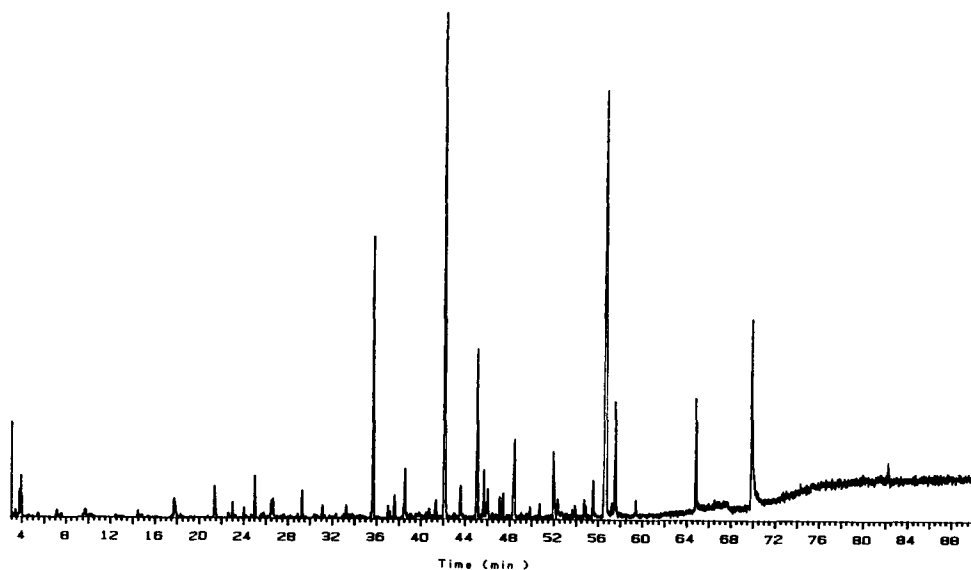


Fig. 2. TIC trace of hydrofluorosilicic acid extract (for GC-MS operating conditions see text).

on a different spectrometer. In addition to the NBS/Wiley data base, a user-created data base consisting of mass spectra acquired on our instrument was also established. Using the search algorithm supplied with the data system it is possible to search these data bases consecutively in a single search.

## RESULTS AND DISCUSSION

The analytical methodology developed in this work has been shown to be applicable to the analysis of trace organic contaminants in inorganic chemicals such as those used by water treatment plants. A sample total ion current (TIC) chromatogram for one of the water treatment chemicals analyzed in this study is given in Fig. 2. As can be seen by the chromatogram, a fairly complex mixture of organic compounds can be extracted from the inorganic matrix. The methods developed for the analysis of water treatment chemicals should be applicable to most other inorganic compounds.

The inorganic chemicals studied in this work are all employed in the water treatment process and were sampled from materials of various suppliers. The role of these chemicals in water purification and their typical application dosages are given

TABLE II  
WATER TREATMENT CHEMICALS

<i>Chemical</i>	<i>Role in treatment process*</i>	<i>Typical dosage (ppm)**</i>	<i>Source</i>	<i>TOC*** (ppm)</i>			
Alum <sup>§</sup> (aluminum sulphate)	Coagulant Coagulant aid	15-150	Alcan (Victoria Harbour, Canada)	1			
			Allied Chemicals (Smith Falls, Canada)	0.9			
			C.I.L. (Ear Falls, Canada)	0.9			
			Allied Chemicals (Valleyfield, Canada)	1			
			Allied Chemicals (Valleyfield, Canada)	6			
Alum	Coagulant Coagulant aid	15-150	Alcan (Huntsville, Canada)	0.2			
			Allied Chemicals (Deseronto, Canada)	0.01			
			Allied Chemicals (Deep River, Canada)	0.01			
			Allied Chemicals (Thorold, Canada)	0.01			
			Diversey (Mississauga, Canada)	0.03			
Ferric chloride	Coagulant Coagulant aid	5-120	Diversey (Mississauga, Canada)	0.03			
			Hydrofluorosilicic acid	Fluoridation	0.6-1.7	C.I.L. (Lampton Works, Canada)	40
						C.I.L. <sup>§§</sup> (Lampton Works, Canada)	20
						C.I.L. (Lampton Works, Canada)	9

TABLE II (continued)

<i>Chemical</i>	<i>Role in treatment process*</i>	<i>Typical dosage (ppm)**</i>	<i>Source</i>	<i>TOC*** (ppm)</i>
Lime <sup>§</sup> (calcium oxide)	pH adjustment Corrosion control Water softening	5-15	Domtar (Beachville, Canada)	300
Polyelectrolytes	Coagulant Coagulant aid	0.05-150	Unknown	0.01
Polyelectrolytes <sup>§</sup>	Coagulant Coagulant aid	0.05-150	Calgon (Toronto, Canada) Allied Colloids (U.S.A.)	0.02 8
Soda ash <sup>§</sup> (sodium carbonate)	pH adjustment Corrosion control Water softening	10-25	Allied Chemicals (Deep River, Canada)	2
Sodium bicarbonate <sup>§</sup>	pH adjustment Corrosion control Water softening	10-30	Allied Chemicals (Amherstburg, Canada) Allied Chemicals (Alexandria, Canada)	0.8 0.04
Sodium hydroxide	pH adjustment Corrosion control Water softening	5-20	C.I.L. (Lindsay, Canada)	0.09
Sodium silicates	Coagulant Coagulant aid Corrosion control	≈ 10	National Silicates (Toronto, Canada)	0.02
Sodium silicofluoride <sup>§</sup>	Fluoridation	0.6-1.7	National Silicates (Toronto, Canada) Supertos (Owen Sound, Canada)	0.03 1

\* From refs. 11 and 12.

\*\* From refs. 11-14.

\*\*\* Approximate total organic content (TOC).

§ Solid samples.

§§ Same batch as the first hydrofluorosilicic acid sample but passed through a carbon adsorber (manufacturer's cleanup procedure).

in Table II. The total amount of organic constituents found in each sample is also given in Table II. The total organic contents were calculated using an average response factor obtained from the analysis of a standard mixture of compounds analogous to those identified in the water treatment chemicals. The total organic content of the samples analyzed was found to range from 0.01 to 300 ppm. For a given type of chemical there was little difference in the level of the contaminants present even for samples which were obtained from different manufacturers. It was also apparent that aqueous solutions of a given chemical had lower organic contents (in terms of ppm) than their corresponding solid samples. This is not too surprising in that there is a large difference in the weights of the solutions and solids which would be required to give the same dosage of the desired inorganic compound. However, because the concentrations of these solutions were not supplied, it is impossible to determine if

TABLE III

## COMPARISON OF COMPOUNDS IDENTIFIED IN SOLID ALUM SAMPLES

Samples: alum No. 1, Alcan (Victoria Harbor); alum No. 2, Allied Chemicals (Smith Falls); alum No. 3, C.I.L. (Ear Falls); alum No. 4, Allied Chemicals (Valleyfield); alum No. 5, Allied Chemicals (Valleyfield).

Compound	Mol. wt.	Sample No.				
		1	2	3	4	5
Methylcyclopentane	84			x		
Cyclohexanone	98		x		x	x
Formic acid, cyclohexyl ester	128			x		
Nonanal	142			x		
Cyclohexanol	100		x		x	
2-Hexen-1-ol	100					x
Dihydro-5-methylfuranone	100			x		
2-Chlorocyclohexanone	132			x		
Dihydro-5-ethylfuranone	114			x		
8-Chloro-1,4-dioxaspiro[4,5]decane	176			x		
Dihydro-5-propylfuranone	128			x		
Cyclododecane	168		x			
Dihydro-5-butylfuranone	142			x		
Dodecanol	186	x	x			
Dihydro-5-amyfuranone	156			x		
Isopropyl myristate	270	x				
Hexanoic acid	116					x
Butanoic acid, hexyl ester	172					x
Heptanoic acid	130					x
Octanoic acid	144				x	x
Nonanoic acid	156				x	x
1,2-Benzenedicarboxylic acid, diethyl ester	222	x				x
1,3,5-Tri-2-propenyl-1,3,5-triazine-2,4,6-trione	249	x	x			
Decanoic acid	172				x	x
1,3-Di- <i>tert.</i> -butyl-2-hydroxy-5-methylbenzene	234		x			
Octadecanol	270	x				
Nonanedioic acid, dibutyl ester	300			x		
Docecanoic acid	200				x	x
1,2-Benzenedicarboxylic acid, dibutyl ester	278	x	x			
Undecanedioic acid, dibutyl ester	328			x		
Tetradecanoic acid	228				x	x
Pentadecanoic acid	242					x
Hexanedioic acid, dioctyl ester	370					x
Hexadecanoic acid	256				x	x
Heptadecanoic acid	270				x	x
Octadecanoic acid	284				x	x
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	390	x	x	x		x
1,2-Benzenedicarboxylic acid, diisooctyl ester	390					x
1,2-Benzenedicarboxylic acid, dioctyl ester	390					x
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	312	x	x			x

the total organic content relative to the actual amount of the inorganic compound is approximately equal for the solid and liquid alums, for example. Some water treatment plants are equipped to utilize solutions of these chemicals while other plants may find it more convenient to work with the solid materials.



TABLE IV

## COMPARISON OF COMPOUNDS IDENTIFIED IN LIQUID ALUM SAMPLES

Samples: alum No. 1, Alcan (Huntsville); alum No. 2, Allied Chemicals (Deseronto); alum No. 3, Allied Chemicals (Deep River); alum No. 4, Allied Chemicals (Thorold).

Compound	Mol wt.	Sample No.			
		1	2	3	4
Cyclohexanone	98			x	
Cyclohexanol	100		x	x	
3-Methyl-2-furanone	98		x	x	
3-Methyl-2-norcaranone	124		x		
Ethylcyclohexane	112		x	x	
Undecanol	172	x			
2-Methyl-1-penten-3-one	98		x	x	
Sulfonylbismethane	94		x	x	
Phenol	94				x
Branched alcohol (C <sub>14</sub> H <sub>30</sub> O)	214	x			
Tetrahydropyran-2-ol	102				x
Branched alcohol (C <sub>16</sub> H <sub>34</sub> O)	242	x			
1-Isobenzofuranone	134		x	x	
1,2-Benzenedicarboxylic acid, diethyl ester	222		x	x	x
Heptanedioic acid, dibutyl ester	272	x			
1,3,5-Tri-2-propenyl-1,3,5-triazine-2,4,6-trione	249	x	x	x	x
Branched alcohol (C <sub>18</sub> H <sub>38</sub> O)	270	x			
3,3'-Oxybispropanenitrile	124			x	
Nonanedioic acid, dibutyl ester	300	x			
Octadecanol	270			x	
Branched alcohol (C <sub>20</sub> H <sub>42</sub> O)	298	x			
1,2-Benzenedicarboxylic acid, dibutyl ester	278	x	x	x	x
4-Hydroxybenzaldehyde	122				x
Undecanedioic acid, dibutyl ester	328	x			
Branched alcohol (C <sub>22</sub> H <sub>46</sub> O)	326	x			
Tridecanedioic acid, dibutyl ester	356	x			
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	390	x	x	x	x
1,2-Benzenedicarboxylic acid, diheptyl ester	362				x
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	312		x	x	x
1,2-Benzenedicarboxylic acid, dioctyl ester	390				x
1,2-Benzenedicarboxylic acid, dinonyl ester	418				x
1,2-Benzenedicarboxylic acid, didecyl ester	446				x

Tables III-VIII list the organic contaminants which were identified in some of the water treatment chemicals analyzed. The organic contaminants which were identified consisted of compounds such as: straight-chain alkenes, alcohols, and carboxylic acids; aliphatic and phthalate esters; cyclic ketones, alcohols, and alkenes; phenolic compounds and other substituted aromatic compounds; and compounds containing nitrogen and/or sulphur. Almost all of these constituents are simple compounds containing only carbon, hydrogen, and oxygen atoms, while chlorinated compounds are virtually absent with only three being identified. This is a significant fact because many chlorinated species have a high toxicity and therefore their presence is very undesirable. Although there were a wide variety of water treatment chemicals

TABLE V  
COMPARISON OF COMPOUNDS IDENTIFIED IN POLYELECTROLYTES

Samples: polyelectrolytes No. 1, unknown source; polyelectrolytes No. 2, Calgon (Toronto, Canada); polyelectrolytes No. 3, Allied Colloids (U.S.A.).

Compound	Mol. wt.	Sample No.		
		1	2	3
Octanol	130			x
Decanoic acid, methyl ester	186			x
Hexadecene	224			x
Decanol	158			x
Dodecanoic acid, methyl ester	214			x
Octadecene	252			x
Tetradecanoic acid, methyl ester	242			x
2-Propenamide	71	x		
Hexadecanoic acid, methyl ester	270			x
Tetradecyne	194		x	
1,1'-[Oxybis(methylene)]bisbenzene	198			x
5-Ethyl-2-methyl-5-hepten-3-one	154	x		
Octadecenoic acid, methyl ester	296			x
Benzoic acid, phenylmethyl ester	212			x
3,3'-Oxybispropanenitrile	124	x		
3,3'-Iminobispropanenitrile	123	x		
1,2-Benzenedicarboxylic acid, dibutyl ester	278	x		x
Hexadecanoic acid	256	x		
Hexanedioic acid, dioctyl ester	370		x	
Octadecanoic acid	284	x		
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	390	x		x
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	312	x		
Spectra-sorb UV 531 (C <sub>12</sub> H <sub>26</sub> O <sub>3</sub> )	326			x

TABLE VI  
COMPARISON OF COMPOUNDS IDENTIFIED IN SODIUM SILICATES SAMPLES

Samples: sodium silicates No. 1, National Silicates (Toronto, Canada); sodium silicates No. 2, National Silicates (Toronto, Canada).

Compound	Mol. wt.	Sample No.	
		1	2
2,6-Bis(1,1-dimethylethyl)-4-methylphenol	220	x	
Pentanedioic acid, dibutyl ester	244		x
Hexanedioic acid, dibutyl ester	258		x
1,2-Benzenedicarboxylic acid, diethyl ester	222	x	
Heptanedioic acid, dibutyl ester	272		x
1,3,5-Tri-2-propenyl-1,3,5-triazine-2,4,6-trione	249	x	
Octanedioic acid, dibutyl ester	286		x
Nonanedioic acid, dibutyl ester	300		x
1,2-Benzenedicarboxylic acid, dibutyl ester	278	x	x
Undecanedioic acid, dibutyl ester	328		x
Hexanedioic acid, dioctyl ester	370		x
2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene	410	x	
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	390	x	x
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	312	x	x

TABLE VII  
COMPARISON OF COMPOUNDS IDENTIFIED IN SODA ASH SAMPLES

Samples: soda ash No. 1, Allied Chemicals (Deep River); soda ash No. 2, Allied Chemicals (Amherstburg).

Compound	Mol. wt.	Sample No.	
		1	2
Chloroform*	118	×	×
Toluene	92	×	×
2-Ethyl-1-hexanol	130	×	
2-Methyl-2,4-pentanediol	118	×	
1-(2-Butoxyethoxy)ethanol	162	×	
Dodecanol	186	×	×
1-Methyl-bis(2-methylpropyl)thiobenzene	236	×	
Di- <i>tert.</i> -butylhydroxyanisole	236	×	×
Tetradecanol	214	×	×
Octadecanol	270		×
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	390		×
Octadecanoic acid	284	×	
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	312		×

\* Impurity in the dichloromethane.

studied, there were many organic compounds or compound classes which appeared in several different chemicals. It is possible that these compounds may be introduced into the water treatment chemicals during their manufacturing, packaging, or transportation. One of the most commonly occurring compound classes are the phthalate esters which are found in many environmental samples<sup>15</sup>. Because of their ubiquitousness in the environment, special care must be taken to ensure that they are not introduced into the sample during the preparation procedure.

It is also interesting to note that when two samples were obtained from the same supplier, there are many organic contaminants which could be identified in both samples. However, when samples of the same chemical were obtained from different suppliers there are differences in the types of contaminants present. This tends to support the previously suggested explanation for the occurrence of the organic contaminants in the water treatment chemicals.

Two of the hydrofluorosilicic acid samples which were analyzed consisted of samples which were taken from one batch with one being subjected to the manufacturer's cleanup procedure and the other remaining untreated. This cleanup reduced the total organic content by 50%, although it is interesting to note that some of the compounds appeared to be very effectively removed while others were only slightly reduced in quantity. Therefore the cleanup procedure shows some selectivity towards certain compounds in terms of the amount of contaminant which is removed.

Another important consideration is the amount of organic contaminants introduced into the water supply through the application of these various treatment chemicals. The chemicals studied were found to contain parts per million (ppm) or parts per billion (ppb)\* levels of organic contaminants. Since the chemicals themselves

\* Throughout this article the American billion ( $10^9$ ) and-trillion ( $10^{12}$ ) are meant.

TABLE VIII

## COMPARISON OF COMPOUNDS IDENTIFIED IN HYDROFLUOROSILICIC ACID

Samples: hydrofluorosilicic acid No. 1, C.I.L. (Lampton Works); hydrofluorosilicic acid No. 2, C.I.L. (Lampton Works) (same batch as the first sample but passed through a cleanup procedure by the manufacturer); hydrofluorosilicic acid No. 3, C.I.L. (Lampton Works).

<i>Compound</i>	<i>Mol.</i> <i>wt.</i>	<i>Sample No.</i>		
		<i>1</i>	<i>2</i>	<i>3</i>
2,4,6-Trimethyloctane	156	×	×	×
Branched alkane (C <sub>11</sub> H <sub>24</sub> )	156	×		
Acetic acid	60	×	×	×
Propanoic acid	74	×	×	×
2,2-Dimethylpropanoic acid	102		×	×
Butanoic acid	88			×
3,4-Dimethyl-2,5-furandione	126	×		
Pentanoic acid	102			×
4,5,5-Trimethyl-2-furanone	126	×	×	×
3-Ethyl-4-methyl-3-penten-2-one	126		×	
1-Cyclohexylethanone	126	×		
Hexanoic acid	116			×
2,3-Dimethyl-2-butenic lactone	112	×	×	
2,6-Bis(1,1-dimethylethyl)-4-methyl-phenol	220	×		×
Cyclododecane	168	×		×
Di- <i>tert.</i> -butylhydroxyanisole	236	×	×	×
2-Hydroxy-3,5,5-trimethyl-2-cyclohexenone	154	×		
Hexadecyloxyethanol	286		×	
Benzoic acid	122	×		×
1-Methyl-2,4-dinitrobenzene	182	×		
3-Methylbenzoic acid	136			×
Benzenoacetic acid	136			×
Octadecanol	270	×	×	×
Eicosatriene	276		×	×
Tetradecanoic acid	228		×	
Hexadecanoic acid	256	×	×	×
Octadecanoic acid	284	×	×	×

are typically applied in ppm dosages, the resulting concentration of organic compounds in the water supply will be parts per trillion (ppt) or less. Government regulations have established maximum acceptable limits of various organic contaminants at either ppm or ppb levels. Thus the amount of organic compounds introduced into the water supply through the use of water treatment chemicals is relatively insignificant.

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