Int. J. Chem. Sci.: 11(3), 2013, 1321-1326
ISSN 0972-768X
www.sadgurupublications.com

DETECTION OF ORGANICS BY FTIR AND GC-MS

S. V. MAHAJAN[*] and V. S. SHRIVASTAVA[a]

Smt. Sharchchandrika Suresh Patil Institute of Technology (Polytechnic), CHOPDA – 425107, Dist.: Jalgaon (M.S.) INDIA
[a]Nano Chemistry Research Laboratory, G. T. P. College, NANDURBAR – 425412 (M.S.) INDIA

ABSTRACT

Dichloromethane extracted samples of the ground water collected from area of Shirpur city (Maharashtra) were recorded for IR and GC-MS. Several organic compounds have been found. These compounds ultimately affect the soil and ground water quality of the area.

Key words: FTIR, GC-MS, Ground water, Shirpur.

INTRODUCTION

There are several types of pesticides used in Shirpur. This initiates the necessity to monitor the groundwater quality in terms of the concentration of organics. The sorption of pesticides by solid material and its resulting influence on its biodegradation is also important to be taken into consideration, when measuring its impact on the groundwater.

Research is required to measure the concentration of toxic substances such as pesticides that affect human health, mainly those that need time for biodegradation and depend on environmental conditions such as soil composition, depth to water table, land use and other weathering factors such as temperature, humidity, rainfall intensity and land slope. Several surveys conclude that large quantities of pesticides are used per cultivated crop area. The impact of these pollutants on human health due to their low biodegradability and accumulation of organics.

EXPERIMENTAL

Groundwater samples were collected from the area of Shirpur city. Organic compounds were extracted from these samples by using dichloromethane. Extracted organic

[*]Author for correspondence; E-mail: surenvm@rediffmail.com

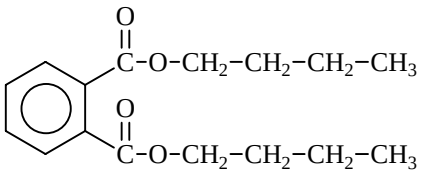
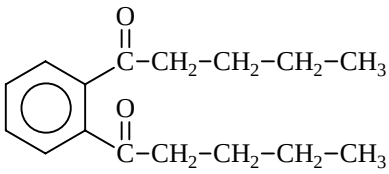
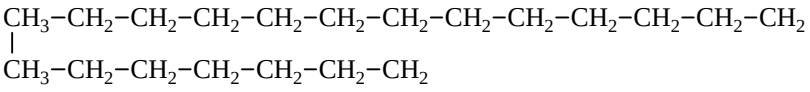
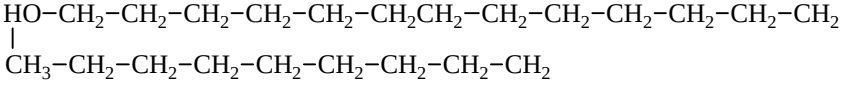
layer was concentrated in small mass. The extracted mass was recorded for FTIR on Perkin-Elmer make IR instrument and GC-MS was recorded on Hewlett-Packard make GC-MS spectrophotometer at Sophisticated Analytical Intrumentation Facility (S.A.I.F.), IIT, Bombay.

RESULTS AND DISCUSSION

The characteristic band IR frequencies were recorded and IR bands support the presence of functional group in detected organic compounds by GC-MS.

The GC-MS spectra of dichloromethane extracted mass were also observed and are in agreement with structures. The identified organic compounds are listed in Table 1 along with their molecular formula and its molecular weight.

Table 1: Chemical compounds found in CH_2Cl_2 extracted mass (Sample-1)

S. No.	Name and structural formula	Molecular formula	Molecular weight
1	Dibutyl phthalate 	$C_{16}H_{22}O_4$	278.34 g/mol
2	Phthalic acid, butyl 2-pentyl ester 	$C_{17}H_{24}O_4$	292.37 g/mol
3	Eicosane 	$C_{20}H_{42}$	282.55 g/mol
4	Behenicalcohol 	$C_{22}H_{46}O$	326.6 g/mol

Cont…

S. No.	Name and structural formula	Molecular formula	Molecular weight
5	1-Docosene $CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2CH_2-CH_2-CH_2-CH_2-CH_2-CH_2$ | $CH_2=CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2$	$C_{22}H_{44}$	308.58 g/mol
6	n-Tetracosanol-1 $HO-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2$ | $CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2$	$C_{24}H_{50}O$	354.65 g/mol
7	Rhodopin (1-hydoxylycopene-1-hydoxy-1,2-dihydrolycopene) | $HO-C-CH_2-CH_2-CH_2-C=CH-CH-CH-C=CH-CH-C=CH-CH=$ | | | | $CH_3-C=CH-CH_2-CH_2-C=CH-CH=CH-C=-CH=CH-C=CH-CH$ | | | |	$C_{40}H_{58}O$	554.89 g/mol

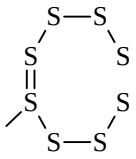
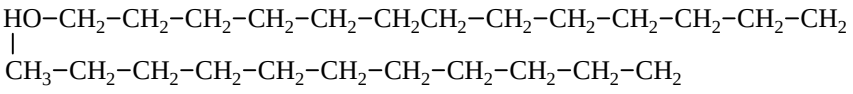
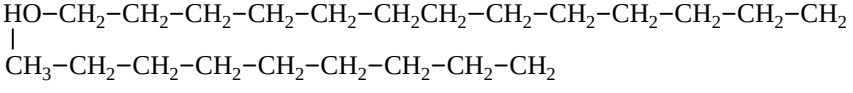
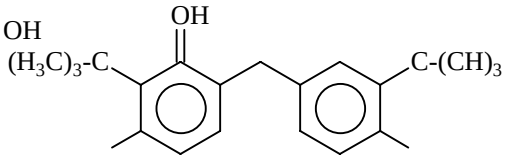
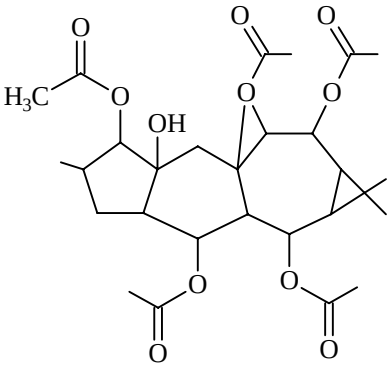
In the early 1960s and 1970s, a considerable effort was expended in protecting and cleaning our surface waters, where the problems of contamination were readily visible. With recent widespread reports of trace quantities of organic pollutants being detected in drinking-water supplies, public attention and regulatory focus has shifted from surface water (lakes and rivers) to groundwater protection. Groundwater contamination has been called the problem of the 1980s.

Toxicity of an organic pollutant is define as its inherent ability to cause an adverse health effect, such as ability to induce cancer, birth defects and other illnesses in animals and humans. The severity of health effects from exposure to organic pollutants is dependentupon the dose (i.e. the magnitude and duration of exposure). For certain chemicals adverse health effects may not be observable at low doses, while death may result from high enough doses. These dose-response relationships are explored earlier[1]. The short-term toxicity of a chemical, manifested over a period of hours or days, is referred to as its acute toxicity. On the other hand, the long-term toxicity, observed after several years of exposure to a chemical, is known as the chronic toxicity.

Acute toxicity is easier to diagnose and treat because the health effects are exhibited over a short period of time and, after exposure to low doses, these effects are usually reversible; that is, when the exposure to the chemical ceases, so do the effects. Among the many organic chemicals that exhibit acute toxicity are: polychlorinated and polybrominated biphenyls (PCBs and PBBs), a group of chemicals that are used in paints, electrical

trasformers, and insulators; and the pesticides aldicarb, parquet, and DDT. Some of the acute effects from exposure to low doses of these compounds include diarrhea, nausea, respiratory distress, vomiting, convulsions, and blurred vision.

Table 2: Chemical compounds found in CH_2Cl_2 extracted mass (Sample 2)

S. No.	Name and structural formula	Molecular formula	Molecular weight
1	Cyclic octaatomicsulfur 	S_8	256.52 g/mol
2	n- tetracosanol-1 	$C_{24}H_{50}O$	354.65 g/mol
3	Behenicalcohol 	$C_{22}H_{46}O$	326.6 g/mol
4	Phenol2,2'-methylene bis (1,1-dimethylethyl)-4-methyl. 	$C_{23}H_{32}O_2$	340.499 g/mol
5	7 a H-Cyclopenta [a] cyclopropa [f] cycloundecene 2,4,7,7a,10,11-hexol. 	$C_{30}H_{44}O_{11}$	580.66 g/mol

Chronic toxicity is more difficult to diagnose and to treat because in some cases its effects are latent, taking several years before the adverse health effects become evident and by then it may be too late to reverse or terminate the adverse effects. Because of the uncertainty of affliction and the protracted effects, it is the chronic toxicity of organic pollutants in drinking water that is the major concern of scientists and the public. On the basis of their chronic toxic effects, organic chemicals may be grouped into the following three major classes: carcinogens, mutagens, and teratogens.

Any chemical that causes cancer in either a direct or an indirect form is called a carcinogen. Although carcinogenesis is the most studied of all chronic effects, it is not entirely clear as to how carcinogens cause cancer. It is known, however, that these chemicals cause or stimulate the formation of malignant tumers of various forms in many parts of the body. Fewer than 30 agents are definitely linked to cancer in humans. In contrast, nearly 1,500 agents are reported as being carcinogenic in animal tests, although this number includes the results from studies with questionable experimental design. Only about 7,000 of the over 5 million known substances have been even tested for carcinogenicity.

Among the chemicals suspected to produce carcinogenic effects in humans are: vinyl chloride, a component of some resins used in construction; benzene, a product of petroleum refining and used as a solvent; and benzo (a) pyrene, a constituent of coal, kerosene, and shale, as well as a naturally occurring chemical in many raw and cooked foods. Numerous other chemicals, including the pesticides ethylene dibromide (EDB), kepone, heptachlor, and dieldrin, are known to produce cancer in animals.

A chemical capable of producing an inheritable change in the genetic material is called a mutagen. We know little about the mutagenic effects of organic chemicals. Most of the chemicals suspected to be mutagenic have only been tested using microorganisms and animals. Chemicals that have been found to be mutagenic include: vinyl chloride; benzo (a) pyrene, bromoform; chlorodibromomethane; and the fungicides folpet and captan.

Any chemical that acts during pregnancy to produce a physical or functional defect in the developing offspring is known as a teratogen. Scientific knowledge on teratogens is very limited. Some of the chemicals that have been shown to have teratogenic effects in animals are: nicotine, found in cigarettes; and the pesticides 2, 4- D, 2,4,5-T, and folpet. It is important to recognize that studies based only on animal species are not always accurate in determining human teratogens.

Besides the major types of health effects discussed above, there are other effects. They include: arteriosclerosis; various forms of heart diseases; hypertension; emphysema;

bronchitis; kidney and liver dysfunction; and diabetes. There is some evidence which links certain organic chemicals to metabolic disorders that stimulate abnormal production of enzymes[2-9].

ACKNOWLEDGEMENT

Authors are thankful to the Head, S. A. I. F., IIT, Bombay.

REFERENCES

1. P. S. C. Rao, M. P. Rao and B. S. Anderson, Organic Pollutants in Groundwater : 2. Risk Assessment, Soil Sci. Fact Sheet SL 55, Institute of Food & Agric. Sci., Univ. of Florida, Gainesville, FL (1987).
2. A. G. Hornsby, Groundwater: Ahidden Resource, Soil Sci. Fact Sheet SL 48, Institute of Food & Agric.Sci., Univ. of Florida, Gainesville, FL (1986).
3. S. Boyd, A. Jones, A. Knaus and C. McGrath (Editors), Drinking Water: A community Action Guide. Concern, Inc., Washington, DC. 30 pages (1986).
4. D. Z. Haman and D. B. Bottcher, Home Water Quality and Safety, Extension Circular 703, Institute of Food & Agric. Sci., Univ. of Florida, Gainesville, FL. (1986) p. 12.
5. P. S. C. Rao, R. S. Mansell, L. B. Baldwin and M. F. Laurent, Pesticides and their Behaviour in Soils and Water, Soil Sci. Fact Sheet SL 40 (Revised), Institute of Food & Agric. Sci., Univ. Florida. Gainesville, FL. (1983) p. 4.
6. National Academy of Sciences, Drinking Water and Health, Chapter 6, **Vol. 1**, National Academy of Sciences, Washington, DC (1977).
7. C. C. Travis and E. L. Etnier (Editors), Groundwater Pollution : Environmental and Legal Problems, Amer. Assoc. for Advancement of Science (AAAS) Selected Symposia Series 95, Westview Press, Inc., Boulder, CO. (1984) p. 149.
8. M. Pice, Introducing Groundwater, George Allen & Unwin (Publishers) Inc., London, UK. (1985) p. 195.
9. U. S. EPA, Pesticides in Groundwater: Background Document, Office of Groundwater Protection, U.S. EPA, Washington, DC. (1986.) p. 72.

Revised : 03.04.2013 *Accepted : 06.04.2013*