



IDENTIFICATION OF ORGANIC COMPOUNDS IN GROUND WATER SAMPLES BY FTIR AND GC-MS

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ABSTRACT

Dichloromethane extracted samples of the ground water collected from area of Shindkheda 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, Shindkheda.

INTRODUCTION

Phenolic compounds are a group of organic pollutants present in the environment as a result of various processes such as industrial, biogeochemical and pesticide degradation. These compounds especially chlorophenols are known for their toxicity and persistence in the environment. They are also accumulative, due to their oleophilicity. These are harmful to living beings, if present in low concentration. For these reasons, some of them have been included in the list of priority pollutants of several countries and are subject to legislation^{1,2}. Toxicity and bioaccumulative potential of chlorophenols increase with the degree of chlorination³, chlorophenol lipophilicity⁴ and the number of chlorine substituents on the phenolic ring¹.

The toxic effects of chlorophenols seem to be linked to a chain reaction of their gradual dechlorination in body fluids and the formation of free radicals interfering with subcellular structures. The formation of peroxides and other products of lipid oxidation result in enzyme deactivation and liver dystrophy. Chronic toxicity studies on carcinogenic properties of some chlorophenols indicate that higher chlorophenols have immunosuppressive effects, are nephrotoxic and interfere with blood formation.

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EXPERIMENTAL

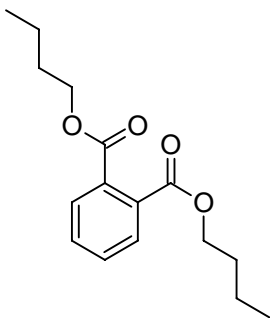
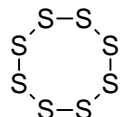
Groundwater samples were collected from the area of Shindkheda city. Organic compounds were extracted from these samples by using dichloromethane. Extracted organic layer was concentrated in small mass. The extracted mass was recorded for FTIR on Perkin-Elmer make IR instrument and GC-MS was recorded on Hewlett-Packard make GC-MS spectrophotometer at Sophisticated Analytical Instrumentation 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 GC-MS extracted mass (Sample No. 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	Cyclic octaatomicsulfur 	S ₈	256.52 g/mol

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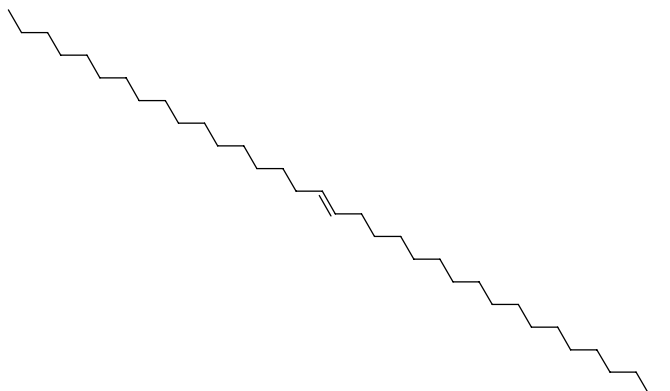
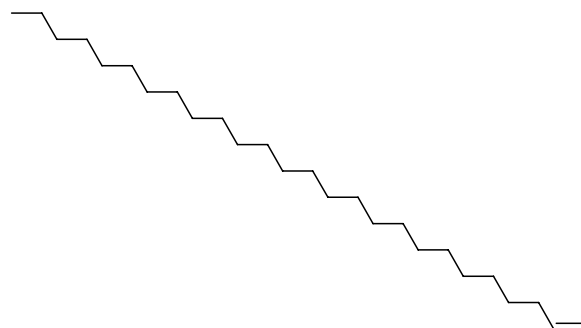
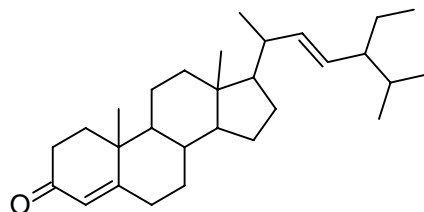
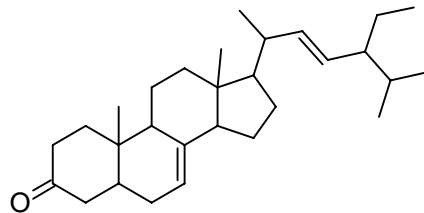
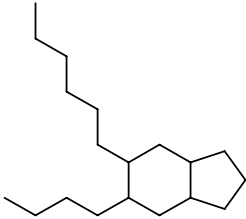
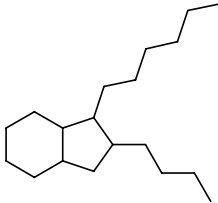
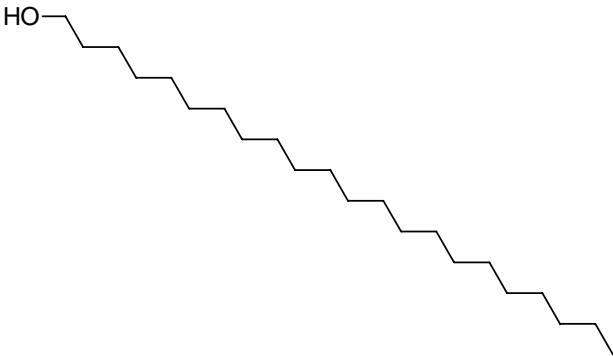
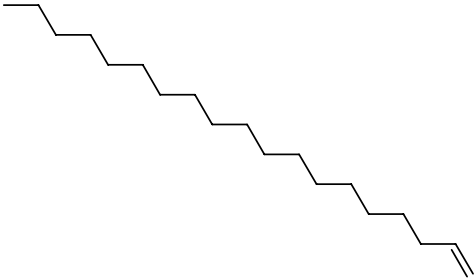
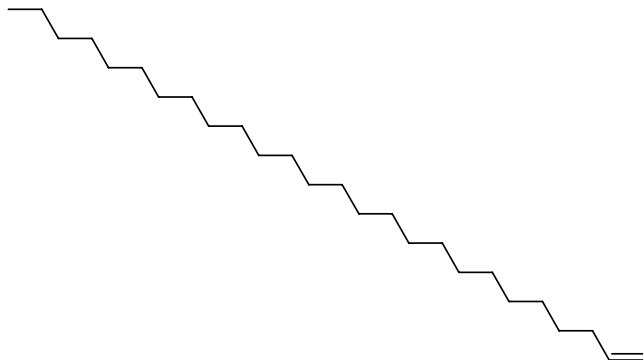
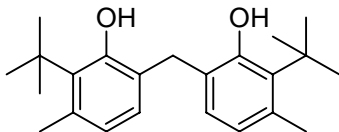
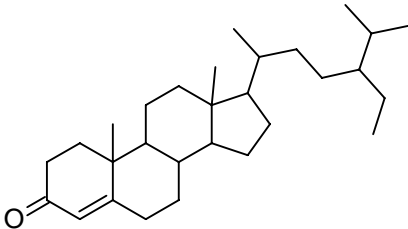
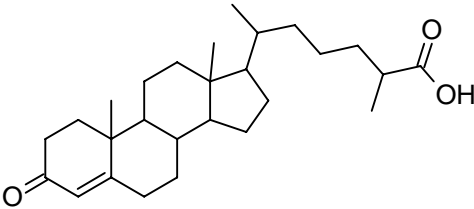
S. No.	Name and structural formula	Molecular formula	Molecular weight
3	17 - Pentatriacontene 	C ₃₅ H ₇₀	490.93 g/mol
4	1 - Hexacosene 	C ₂₆ H ₅₂	364.69 g/mol
5	4, 22-stigmastadiene-3 one 	C ₂₉ H ₄₆ O	410.674 g/mol
6	Spinasterone 	C ₂₉ H ₄₆ O	410.674 g/mol

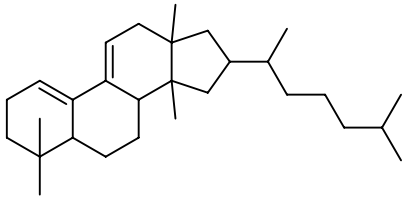
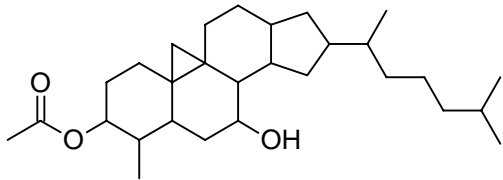
Table 2: Chemical compounds found in GC-MS extracted mass (Sample 2)

S. No.	Name and structural formula	Molecular formula	Molecular weight
1	1 H-Indene-5 butyl-6-hexyloctahydro 	C ₁₉ H ₃₆	264.48 g/mol
2	1-H-Indene-2 butyl-4-hexyloctahydro 	C ₁₉ H ₃₆	264.489 g/mol
3	Behenicalcohol 	C ₂₂ H ₄₆ O	326.6 g/mol
4	1 - Nonadecene 	C ₁₉ H ₃₈	266.51 g/mol

Cont...

S. No.	Name and structural formula	Molecular formula	Molecular weight
5	1 - Hexacosene 	$C_{26}H_{52}$	364.691 g/mol
6	Phenol 2, 2'-methylene bis (1, 1-dimethylethyl)-4 methyl 	$C_{29}H_{48}O$	412.69 g/mol
7	Stigmast 4-en-3 one 	$C_{27}H_{42}O_3$	414.621 g/mol
8	Cholest-4-en 26-oic acid 3-oxo. 	$C_{30}H_{50}$	410.718 g/mol

Cont...

S. No.	Name and structural formula	Molecular formula	Molecular weight
9	3-(1,5-Dimethyl hexyl) 3a, 10,10,12b-tetramethyl 1,2,3,3a,4,6,8,9,10,10a,11,12,12a,12b-tetradecahydrobenzo. 	C ₃₁ H ₅₂ O ₃	472.742 g/mol
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Pesticides are important input to modern agriculture and also used in public health in controlling communicable disease. During the last couple of decades, the use of pesticides has dramatically increased in India. However, the average pesticide consumption India is still one of the lowest in the world at 0.5 Kg/hectare against 10.7 Kg in Japan and 4.5 Kg in the US, mainly because of poor awareness among farmers and high cost of pesticides (Associated Indian Chamber of Commerce and Industry, Mint news, June 2008). The production of pesticides has increased from 5,000 to 85,000 metric tons between the period 1958 and 2004⁵. The toxicity of these compounds poses risk to human health, environment and to the organisms which may not be targeted by pesticides. The effect of pesticides and their mobility depend upon their chemical and physical properties, soil characteristics, groundwater infiltrations and vadose zone behaviour, vegetation and local weather conditions. They resist degradation by chemical, physical and biological means. The degradation of DDT in soil is 75 to 100% in 4 to 30 years⁶⁻⁸.

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