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Pollution of Moscow air in winter: a GC-MS study of snow samples

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Abstract

To find the most common and dangerous organic pollutants in the winter atmosphere of Moscow 4 snow samples were collected in various places in the city. Two "clean" samples from arctic territories of Finland and one from Baikal region in Siberia were collected as background. These samples were also used to detect possible atmospheric transportation of pollutants to the cold regions of the Earth. GC-MS was used as an analytical tool to identify and quantify individual organic compounds belonging to the various classes. As a result more than 250 compounds were detected. The possible presence of more than 100 other priority pollutants from the US EPA list was also screened.

Introduction

Being one of the major cities of the world Moscow is a big industrial territory. Thousands of various chemicals appear every day in the air of the city due to emissions of plants, transportation, power stations, etc. Environmental laboratories regularly screen the presence of the well-known atmospheric pollutants (mainly inorganic). On the other hand the list of the priority pollutants is not composed yet. Thus the main task of the work was to select the most important compounds to start the composition of the priority pollutants list. The idea was to collect snow in spring to elucidate the overall

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amount of pollutants transported by air during winter period [1]. The freshly fallen snow usually do not contain any pollutants [2]. Actually analysis of snow samples is quite useful approach for mapping of territories to compare health problems of the population with the qualitative and quantitative composition of the atmosferic organic and inorganic pollutants. It was successfully aplied during last 20 years in various regions of Russia [3-6].

To study this problem using GC-MS detection of organophosphorus pesticides, persistent organochlorine pesticides, PCBs, phenols, PAH, and some other priority pollutants the samples of snow were collected in Moscow and in "clean" regions of the world Lapland and at lake Baikal.

Materials and methods

The snow samples were collected in early March from: 1. Muonio (Lapland, Finland), 2. Levi (Lapland, Finland), 3. Butovo (clean city area, southern end of Moscow, Russia), 4. Moscow State University (clean city area, Moscow, Russia), 5. Shosse Entuziastov (heavy industrial district, Moscow, Russia), 6. Moscow region - summer cottage area, and 7. Baikal'sk on Lake Baikal, (Siberia). Snow samples were kept in polyethene bags and transported on ice to the laboratory. Melted snow (1 l) was saturated at room temperature with solid NaCl. To extract the base/ neutral pollutants, 60 ml dichloromethane was added to the samples adjusted to pH 11 by NaOH (1N), shaken to rinse also the inner surface and transferred to the separatory funnel (for 2 liters). The funnel was shaken for 15 min. with periodic venting to release excess pressure. After the layers were separated, the dichloromethane extract was collected into a 250 ml flask. The procedure was repeated three times i.e. finally 180 ml of the dichloromethane extract were obtained.

For the extraction of acidic pollutants the pH of the aqueous phase was adjusted to 2 using 1 N solution of sulfuric acid. Extraction procedure was the same as for the neutral and basic compounds. Both base/ neutral and acid fractions were separately dried over anhydrous sodium sulfate and concentrated in Kuderna-Darish concentrator to reach final volume of 1 ml. Just prior to the GC-MS analysis, the base/neutral and acid extracts were combined.

Three internal standards were used during the analysis of the samples (D_8 - naphtalene, D_{10}-phenananthrene and D_{12}-perylene). These internal standards covered the range of the masses and retention times of the compounds of interest, while response factors calculated on their bases satisfy the requirements of the US EPA method 8270 for the semivolatile priority pollutants.

Hewlett-Packard 5989 "Engine" GC-MS system was used. The following parameters were applied during the analyses: mass range 25-550 amu, scanning rate - 0.5 sec, ionization energy - 70 eV (electron impact), chromatographic column 30 m x 0.53 mm x 1.5 μm HP - 5, temperature

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program: Initial temperature 50°C 4 min., gradient 8/min., final temperature 300°C (20 min.).

The software provided by Hewlett-Packard enabled to reconstruct Extracted Ion Current Profiles (EICP) and allow integration of the abundances in any EICP between specified time or scan limits. The Wiley mass spectra library for 275,000 compounds of the software was used for the qualitative analysis.

Results and discussion

The results obtained during the present study are summarised in Tables 1-11. The results on organophosphorus pesticides (Table 1) appeared quite unexpected, since the only sample containing several representatives of this class of chemicals was from Lake Baikal (sample 7 Table 1). Since this region is considered to be rather clean we did not expect such results. These compounds characterize agricultural contamination. Diazinon and pirimifos methyl are not used in Russia, on the other hand these pesticides are widely spread in China. There is only limited agriculture in Baikal'sk area. Organophosphate fenitrothion was also detected in Finnish samples from Lapland. Agriculture is again minimal in this area and the local use of organophosphates is not probable. The levels in Lapland were less than in Baikal'sk. Probably fenitrothion represents again long distance transportation. These facts may indicate "cold finger" effect. We also add to the Table tributyl- and triphenylphosphates as the compounds containing phosphorus.

Organophosphorus pesticides are known to be base-degradable. To estimate the losses during sample preparation the matrix spike sample was analysed. Eight organophosphorus pesticides (standards) were added to the snow sample 1 and complete sample preparation procedure followed by the GC-MS analysis was carried out. The recoveries were as follows: Chlorpyriphos-methyl -70 %, Diazinon -53 %, Dichlorvos -0 %, Fenitrothion - 64 %, Malathion 24 %, Methacrifos- 100 %, Phosphamidon- 0 %, Pirifimiphos-methyl -30 %. The data obtained indicate that some organophosphates are quite resistant, but some are very sensitive. Thus we may have lost some components.

Only 3 organochlorine pesticides or their metabolites were detected in trace amounts in the samples studied (Table 2). Again the Baikal'sk sample appeared to be contaminated. The other organochlorines, first of all PCB, were found in trace amounts in some of the Moscow samples (Table 2). The obvious leader in the levels of these compounds is the sample collected in the region of the Moscow State University. Probably this contamination involves some unregistered waste releases from the laboratories of Chemical and Biological Departments of the Moscow State University where experiments with these compounds are carried out.

Petroleum hydrocarbons (alkanes) usually appear to be the most common group of environmental pollutants (Table 3). We identified and quantified from

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the snow samples 47 compounds of this class in the range between nonane (C_9) and hexatriacontane (C_{36}). The maximal levels in this group were of C_{18}-C_{33}. These hydrocarbons belong to the high boiling petroleum fractions (lubricating oils and paraffins). Surprisingly Finnish sample from Levi (downhill skiing resort in Lapland) was the most contaminated. Amount of these pollutants even in industrialized Moscow areas (samples 4 and 5) was lower. Taking into account that petroleum hydrocarbons are easily photo- and biodegradable it is hardly possible that transboundary transfer could be the cause of contamination of Finnish territory at the sampling places with these chemicals. Most probably they have originated from the heavy vehicles, used to clean the roads from snow. Maximal allowable concentration (MAC) value in Russia for the sum of petroleum hydrocarbons in surface water basins is 50 μg/l. Thus the concentration of these compounds in the melted snow in Levi area exceeded this value in 3.6 times. Diesel engines as well as burning candels may be suspected to be a possible source of these pollutants in Lapland.

Fatty acids is another large group of organic compounds present in environment. The source of these chemicals is the degradation of hydrocarbons and hydrolysis of fats. The total amount of these compounds in the samples does not differ significantly (Table 4). Fatty acids are not considered to be dangerous, and their maximal allowable concentration values are quite high.

Phthalates are included into priority pollutant lists in many countries. They are used as plasticisers and they are rather stable and widely spread all over the world. They may be found almost in every environmental sample. Dibutyl- and bis-(2-ethylhexyl)phthalates are the most widely used representatives of this class of chemicals. The results obtained demonstrated serious contamination of snow with these compounds (Table 5). In fact the value of MAC for dibutylphthalate (1μg/l) is exceeded in all the samples. Butylbenzylphthalate is not typical for Russia. The results obtained proved this fact. This compound was present in significant concentrations in Finnish samples, while only 2 Russian samples were contaminated at lower levels. The only exception is sample 5, collected in extremely industrialized area in the middle of Moscow.

A group of priority organic pollutants (US EPA list) detected in the samples are represented in Table 6. To discuss these results is not easy, since various pollutants were detected in various samples.

Phenols constitute another group of environmental pollutants included into the international priority lists. The results summarized in Table 7 demonstrate rather low levels of these contaminants in the snow. Only in case of sample 5 (the most industrialized region of Moscow) the concentration of phenol exceeded the MAC level (1 μg/l). There were no priority chloro- or nitrophenols observed in any of the samples studied.

Polycyclic aromatic compounds (PAH) are of major concern in environmental legislations all over the world. The main source of their penetration into environment involves fuel combustion. The results obtained

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(Table 8) may be considered as quite encouraging, with the only exception of 3 Russian samples (including one from Baikal'sk) where the most hazardous benz[a]pyrene was found. In fact, *a priory*, we expected higher levels of these compounds. Again sample 5 holds a record. Concentration of PAH in this sample was one order of magnitude higher than in others. The most reasonable source of this phenomenon is incomplete combustion of oil (cars, factories, power plant etc.). This observation is supported by the fact that this sample was more rich with higher representatives of this group than other samples.

Table 9 contains the information on concentration of antioxidants, their by-products and metabolites in the samples. All the samples from Moscow were contaminated to some extent with compounds of this group. These purely antropogenic contaminants were absent in all the samples from Finland. Only the main representative of this group 2,6-di-tert-butyl-4-methylphenol was detected everywhere. In fact, this compound may be found almost in every environmental sample collected anywhere in the world.

Table 10 contains the results on the presence of natural compounds in the snow samples. They are not known to be hazardous. The highest levels of these compounds were detected for Finnish samples and that from Baikal'sk region. This result is pretty expectable since forest is their main source. The only exception involves the hopane group (triterpanes) identified in sample 5. These substances constitute a heavy fraction of the crude oil. The most reasonable source of their appearance in Moscow is asphalt. The road works carried in winter time at this place could cause an evaporation of these products from the hot asphalt and their deposition in snow.

Table 11 contains miscellaneous organic pollutants belonging to the most different classes of organic compounds (alcohols, amides, aldehydes, ketones, esters, etc.). These compounds do not belong to the lists of priority pollutants since their toxicities are not high or unknown and they are not spread over the vast territories. Russian samples were richer in these pollutants than the Finnish ones. However, the Finnish sample 2 was characterized with quite high levels of some of them. Very high concentrations of some amides were detected for sample 5. Again as with surfactants industrial enterprises of the region should be in charge of their origin.

Eleven surfactants (64.9μg/kg) belonging to polyethyleglycoles were detected only in sample 5. They could arise from one of enterprises.

Besides these compounds (Tables 1-11) nineteen chemicals remained unidentified due to poor matches with the libraries of mass spectra.

Conclusions

1. More than 250 organic compounds were identified in 10 snow samples collected in March 1998 in Finland and Russia. The presence of about 100 other hazardous pollutants was screened, but they were not detected.

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2. The first portion of data to create Moscow list of atmospheric priority pollutants was obtained.
3. The snow samples of Lake Baikal area contained significant amounts of organophosphates, which are not used in Russia and this indicates long distance transportation from southern agricultural areas. The presence of organochlorines in Lake Baikal area confirms this conclusion.
4. The levels of phenols and PAH in all the samples were lower than it had been expected on the basis of the former experience.

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Table 1. Concentration of organophosphorus compounds in the snow samples (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	Methacrifos	-	-	-	-	-	-	0.27
2	Tributylphosphate	-	-	-	-	0.49	-	-
3	Diazinon	-	-	-	-	-	0.04	0.45
4	Chlorpyriphos-methyl	-	-	-	-	-	-	0.06
5	Fenitrothion	0.10	0.10	-	-	-	-	0.60
6	Pirimiphos-methyl	-	-	-	-	-	-	0.26
7	Triphenylphosphate	-	-	-	-	-	-	3.51
	Σ7	0.10	0.10	-	-	0.49	0.04	5.15

Table 2. Concentration of priority organochlorines in the snow samples (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	1,3-Dichlorobenzene	-	-	-	-	0.52	-	-
2	1,4-Dichlorobenzene	-	-	-	-	-	-	0.38
3	1,2,4-Trichlorobenzene	-	-	-	2.60	-	-	-
4	1,3,5-Trichlorobenzene	-	-	-	0.73	-	-	-
5	Endrine aldehyde	-	-	-	-	-	-	0.38
6	DDD	-	-	-	-	-	-	0.02
7	DDE	-	-	0.003	-	-	-	-
8	Tetrachlorobiphenyls*	-	-	-	0.28	-	-	-
9	Pentachlorobiphenyls*	-	-	-	0.77	-	-	-
10	Hexachlorobiphenyls*	-	-	-	0.06	-	-	-
	Σ10	-	-	0.003	4.44	0.52	-	0.78

*The sum of the corresponding isomers

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Table 3. Concentration of petroleum hydrocarbons (alkanes) in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	Nonane	-	-	-	-	-	0.41	-
2	Decane	0.28	0.27	0.06	0.01	-	0.65	-
3	Undecane	0.16	0.17	0.05	0.02	0.16	-	-
4	Dodecane	0.28	0.20	0.05	0.48	0.72	-	-
5	Tridecane	0.22	0.24	0.17	0.55	2.83	-	-
6	Branched alkane	-	-	0.07	-	-	-	-
7	Tetradecane	0.35	0.27	0.19	1.58	5.68	-	-
8	Pentadecane	0.13	0.56	0.12	0.68	0.12	-	-
9	Hexadecane	-	-	0.17	0.04	0.02	-	-
10	Heptadecane	-	0.83	0.09	1.46	1.49	0.59	-
11	Pristane	-	-	-	2.10	1.76	-	-
12	Octadecane	-	0.37	-	0.24	4.57	-	-
13	Phytane	-	-	-	0.29	3.77	-	-
14	Branched alkane	-	1.49	-	-	-	-	-
15	Nonadecan	-	0.77	-	0.85	1.98	0.62	0.04
16	Eicosane	0.19	1.86	-	0.39	0.16	1.20	0.25
17	Heneicosane	0.26	4.56	0.12	0.63	0.12	1.07	1.16
18	Branched alkane	-	1.06	-	-	-	-	-
19	Docosane	0.24	8.48	0.08	0.55	0.98	0.80	0.23
20	Branched alkane	-	0.27	-	-	-	-	-
21	Branched alkane	-	0.63	-	-	-	-	-
22	Tricosane	0.40	13.5	0.12	0.69	0.79	1.87	3.90
23	Branched alkane	-	0.85	-	-	-	-	-
24	Tetracosane	0.44	17.9	0.05	0.39	0.96	1.12	0.56
25	Branched alkane	-	1.61	-	-	-	-	-
26	Pentacosane	0.38	20.1	0.27	0.63	2.58	5.77	3.80
27	Branched alkane	-	0.90	-	-	-	-	-
28	Branched alkane	-	1.10	-	-	-	-	-
29	Hexacosane	0.30	22.6	0.07	1.22	1.01	1.41	0.43
30	Branched alkane	-	1.88	-	-	-	-	-
31	Branched alkane	-	1.06	-	-	-	-	-
32	Heptacosane	0.44	18.3	0.16	2.75	2.92	8.68	1.91
33	Branched alkane	-	1.16	-	-	-	-	-
34	Branched alkane	-	1.05	-	-	-	-	-
35	Octacosane	-	15.4	0.04	1.48	0.95	0.80	0.40
36	Branched alkane	-	0.74	-	-	-	-	-
37	Branched alkane	-	0.70	-	-	-	-	-
38	Nonacosane	-	12.8	0.24	2.36	5.59	5.20	-
39	Branched alkane	-	0.51	-	-	-	-	-
40	Triacontane	-	9.63	-	1.00	-	0.72	-
41	Branched alkane	-	0.41	-	-	-	-	-
42	Untriacontane	-	7.17	-	0.78	-	3.45	-
43	Dotriacontane	-	4.40	-	1.00	-	-	-
44	Tritriacontane	-	2.58	-	0.70	-	-	-
45	Tetratriacontane	-	1.51	-	0.70	-	-	-
46	Pentatriacontane	-	0.95	-	-	-	-	-
47	Hexatriacontane	-	0.42	-	-	-	-	-
	Σ47	4.07	181.2	2.12	23.57	39.16	34.36	12.68

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Table 4. Concentration of fatty acids in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	Hexanoic acid	0.17	0.47	0.11	0.26	-	-	-
2	Heptanoic acid	0.11	0.25	0.03	0.11	-	-	-
3	2-Ethylhexanoic acid	-	0.12	0.14	-	-	-	-
4	Octanoic acid	0.15	0.51	0.06	0.17	-	-	-
5	Nonanoic acid	0.12	0.56	0.05	0.53	-	-	1.51
6	Decanoic acid	0.07	0.36	0.03	0.22	-	-	-
7	Undecanoic acid	-	-	-	0.08	-	-	-
8	Dodecanoic acid	0.07	0.71	0.08	0.34	-	-	-
9	Tridecanoic acid	-	-	0.02	0.11	-	-	-
10	Tetradecanoic acid	0.17	0.75	0.12	0.63	-	-	2.34
11	Iso-pentadecanoic acid	-	-	0.16	-	-	-	-
12	Pentadecanoic acid	0.07	-	0.07	0.21	-	-	-
13	Iso-hexadecanoic acid	-	-	-	0.25	-	-	-
14	Hexadecanoic acid	0.52	1.68	0.38	1.25	0.08	-	2.60
15	Heptadecanoic acid	-	0.1	0.02	-	-	-	-
16	Iso-octadecanoic acid	-	-	-	-	-	-	-
17	Oleic acid	0.10	-	0.14	0.47	2.11	-	-
18	Octadecanoic acid	0.20	0.67	0.14	0.37	-	-	-
	Σ18	1.75	6.18	1.55	5.00	2.19	-	6.45

Table 5. Concentration of phthalates in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	Dimethyl phthalate	0.03	0.09	0.06	0.67	0.51	0.51	0.09
2	Diethyl phthalate	0.06	2.73	0.05	1.99	0.53	0.30	0.39
3	Di-izobuthyl phthalate	0.1	1.15	0.07	3.96	-	0.69	1.26
4	Di-n-buthyl phthalate	3.0	14.9	1.67	31.8	10.85	48.3	52.8
5	Benzylbuthyl phthalate	0.87	0.81	0.07	-	3.05	-	0.17
6	bis(2-Ethylhexyl)phthalate	5.64	9.12	1.30	40.7	19.75	14.5	5.30
7	Di-n-octyl phthalate	0.03	-	-	1.1	1.58	0.78	0.03
8	Decyloctyl phthalate	-	-	-	1.35	-	-	-
	Σ8	9.73	28.8	3.22	81.5	36.27	65.1	60.0

Table 6. Concentration of other priority pollutants (US EPA list) in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	Styrene	-	-	-	-	0.08	-	-
2	Benzaldehide	0.43	0.31	-	0.41	0.14	0.59	-
3	Methylethylbenzene	0.49	-	-	1.18	-	0.75	-
4	Benzyl alchochol	-	-	0.004	0.11	0.04	-	0.30
5	Trimethylbenzene	-		-	-	-	0.35	-
7	Acetophenone	-	-	-	-	0.36	-	-
8	Nitrobenzene	-	-	0.18	-	-	0.47	-
10	Benzophenone	-	-	-	0.20	-	-	-
	Σ10	0.92	0.31	0.184	1.9	0.62	2.16	0.03

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Table 7. Concentration of phenols in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	Phenol	0.004	0.02	0.02	0.21	1.30	-	-
2	2-Methylphenol	-	0.07	-	0.03	-	-	-
3	4-Methylphenol	-	0.04	0.004	0.06	-	-	0.29
4	2,4-Dimethylphenol	-	-	-	0.03	0.05	-	-
5	Ethylphenol	-	0.19	-	-	-	-	-
	Σ 5	0.004	0.32	0.024	0.33	1.35	-	0.29

Table 8. Concentration of Polycyclic Aromatic Hydrocarbons in the samples of snow (μg/kg).

	Compound	1	2	3	4	5	6	7
1	Naphthalene	0.13	0.06	0.01	0.27	0.03	0.39	0.03
2	2-Methylnaphthalene	0.03	0.02	0.004	0.10	-	0.10	-
3	1-Methylnaphthalene	0.03	0.01	0.004	0.11	-	0.10	-
4	Biphenyl	-	0.04	-	0.07	-	-	-
5	Acenaphthylene	-	-	-	0.06	0.11	0.04	-
6	Acenaphthene	-	-	-	-	3.91	0.03	0.45
7	Fluorene	0.01	-	-	0.03	0.10	-	0.08
8	Phenantrene	0.02	0.05	0.01	0.15	1.29	0.16	0.10
9	Anthracene	-	-	-	-	0.15	-	0.10
10	Fluoranthene	0.01	0.85	0.03	0.1	0.86	0.12	0.19
11	Pirene	0.01	0.01	0.002	0.07	0.93	0.07	0.20
12	Benzo[a]antracene	-	-	-	-	1.11	0.02	0.02
13	Chryzene	-	-	-	-	-	0.07	0.02
14	Benzfluoranthene[b,k]	-	-	-	0.03	0.41	-	-
15	Benzo[a]pirene	-	-	-	0.04	0.24	-	0.03
16	Benz[g,h,i]perilene	-	-	-	0.04	0.003	-	-
	Σ16	0.24	0.24	0.06	1.08	9.143	1.1	1.22

Table 9. Concentration of antioxidants and their by-products in the samples of snow (μg/kg).

N	Compound	3	4	5	6	7	8	10
1	2-Sec-butylphenol	-	-	0.3	0.61	-	-	-
2	4-Sec-butylphenol	-	-	0.1	0.79	-	-	-
5	2,6-ditert-butyl-2,5-cyclohedien-1,4-dione	-	-	-	0.07	-	-	4.11
6	2-Tert-butyl-4-methoxyphenol	-	-	0.1		-	-	-
7	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	-	-	-	22.0	45.1	0.99	5.00
9	2,6-Di-tertbutyl-5,6-epoxy-4-methyl-4-hydroxycyclohexanone-1	-	-	-	0.41	-	-	-
10	2,6-Ditertbutyl-5,6-epoxy-4methyl-4-hydroxycyclohexanone-1 (isomer)	-	-	-	3.42	-	-	-
11	2,6-di(tert-Butyl)-4-methylphenol	1.3	6.0	0.1	0.68	13.2	6.76	6.50
12	bis-(sec-butylphenol)	-	-	-	-	-	0.75	-
13	2,6-Di-tert-butyl-4-ethylphenol	-	-	-	-	-	0.92	0.90
15	7,9-Di-tert-butyl-1-oxaspiro-[4,5]-deca-6,9dien-2,8-dione	-	-	-	1.24	-	-	-

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Table 10. Concentration of natural organic compounds in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	α-Pinene	0.29	-	-	-	-	-	-
2	Limonene	0.16	-	-	-	-	-	-
3	Dialkylcyclopentane	0.36	0.09	0.03	0.48	-	-	18.7
4	2-Ethyl-3-methoxy-2-cyclopentenone	-	-	-	-	-	0.31	9.12
5	Kamphene	0.16	0.04	-	-	-	-	-
6	Dialkylcyclopentane	1.31	-	-	2.40	4.60	-	17.7
7	1,2:8,9-Diepoxy-n-mentane	-	-	-	0.55	-	-	-
8	Dialkylcyclopentane (3 isom)	-	-	-	-	-	-	34.6
9	2,4-Dihydroxy-3,6-dimethyl benzoic acid	0.08	1.29	-	-	-	0.54	-
10	Phenanthrenecarboxilic acid derivative	0.79	0.46	-	0.25	-	-	-
11	Squalene	1.14	1.45	1.08	5.56	-	3.36	-
12	28-Nor-17β(H)-hopane	-	-	-	-	3.12	-	-
13	(3β)-Cholest-5-en-3-ol	-	-	-	0.52	-	0.26	-
14	Hopane	-	-	-	0.85	1.27	-	-
15	29-Methylhopane	-	-	-	0.35	0.82	-	-
16	Dimethylhopane (2 isomers)	-	-	-	-	1.15	-	-

Table 11. Concentration of miscellaneous compounds in the samples of snow (μg/kg).

N	Compound	1	2	3	4	5	6	7
1	2-Ethylhexanol	-	0.39	0.08	1.10	-	-	-
2	Octanol-1	-	-	-	0.57	-	-	-
3	Nonanal	-	0.31	0.07	1.74	1.17	-	2.80
4	Decanal	-	0.16	0.01	-	0.39	-	-
5	2-Phenoxyethanol	-	0.28	0.04	-	-	-	-
6	Benzotiazol	-	-	-	0.34	-	0.59	-
7	1(3H)-Isobenzofuranone	0.12	-	-	0.06	5.80	-	-
8	Glicerol triacetate	-	-	-	0.80	-	-	-
9	Ethyl 4-hydroxybenzoate	-	-	-	0.41	-	-	-
10	2-(Nitrophenyl)ethylamine	-	-	0.26	-	-	-	-
11	Tetradecanol-1	-	-	-	-	1.98	-	-
12	N-butylbenzene-sulfonamide	-	2.28	-	-	-	-	-
13	Isopropyltetradecanoate	-	-	-	0.28	-	-	-
14	Cofeine	-	-	-	0.13	-	-	-
15	Hexadecanol-1	0.10	0.36	1.72	0.25	-	-	-
16	Tetradecanamide	-	-	-	-	1.15	-	-
17	Octadecanol-2	-	-	-	-	0.98	-	-
18	Octadecanol-1	0.18	0.41	-	1.07	-	-	-
19	Iso-hexadecanamide	-	-	-	-	9.23	-	-
20	Hexadecanamide	-	-	-	0.41	16.2	-	-
21	Oleoamide	-	-	-	1.96	356	-	-
22	Stearinamide	-	-	-	-	14.7	-	-
23	Isopropylstearate	-	-	0.14	1.58	-	-	-
24	Eicosanol-2	-	-	-	-	3.88	-	-
25	Erucamide	-	-	-	12.9	9.92	-	-