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NEGATIVE ION CHEMICAL IONIZATION MASS SPECTROMETRY - A USEFUL TECHNIQUE FOR THE SELECTIVE DETECTION OF POLAR SUBSTITUTED POLYCYCLIC AROMATIC HYDROCARBONS WITH MUTAGENIC PROPERTIES

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ABSTRACT

Earlier studies have shown that many compounds with toxic properties are able to form stable negative ions. The negative ion mass spectrometric response of polar substances found in indoor air extracts from aluminium smelters was determined and compared with available mutagenicity data. The results indicate that the relationship mentioned above also is valid for polar compounds.

LIST OF CONTENT

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1 INTRODUCTION

The identification of organic compounds with proven or suspected toxic effects is an important condition for the estimation of health impacts of environmental samples. In general two main approaches are applied to identify samples which contain substances with biological effects such as toxicity, carcinogenicity and mutagenicity. The first technique uses biological short term tests (eg. the Ames test) (1) to investigate the mutagenic properties of the sample extract. In many cases information can be acquired whether the sample contain a certain level of mutagenic activity or not. The drawback of this technique is that no specific information is obtained about the nature of the mutagenic compounds. Furthermore, sometimes the extracts are highly cytotoxic and no statement about the mutagenic activity can be made. The second approach, which is frequently used, is identification of single compounds or compound groups with known biological activity using time-consuming preseparation and clean-up steps followed by high resolution gas chromatographic separation combined with mass spectrometric identification. The major drawback of this method is that minor or trace compounds with high biological activity may not be found due to overlap by major compound groups. Furthermore, no additional information is obtainable about the toxic properties of identified compounds which are not investigated earlier by biological tests. There is obviously a need for a technique which links both approaches together. Such a method should be able to identify compounds properly and simultaneously give an indication which of them might have biological effects.

As first outlined by Lovelock (2) and discussed further by Poole (3), there is a certain correlation between electron capture detection response and biological activity of a compound. Included in the term biological activity was toxicity, carcinogenicity, mutagenicity as well as blocking of electron acceptor/donor functions. As an example can be mentioned that only 7 of 114 compounds of the US EPA list of priority pollutants are not significantly electroncapturing (4). Horning and co-workers specified this statement further. They found that toxicity generally is associated with the ability of a compound to form a stable negative ion both by resonance capture and reaction with oxygen (5).

Negative ion chemical ionization (NICI) mass spectrometry has been successfully used to detect selectively carcinogenic polycyclic aromatic hydrocarbons (PAH). Thermal elections were produced using methane as reagent gas. A good correlation between electrons capture attachment and carcinogenic properties were obtained for this compound group (6,7,8).

It was therefore of interest to investigate further if NICI is a suitable method to detect single compounds and compound groups with biological activity with a high degree of selectivity. For this purpose the more polar fractions from air extracts were studied with both electron impact (EI) and NICI mass spectrometry. The samples contained mainly aza-arenes and keto-PAH with known and/or suspected mutagenic and carcinogenic properties as well as other compounds groups without such effects (eg. fatty acids, aliphatic alcohols and amines etc.). Dougherty et al. (9) found that most toxic compounds generally have positive electron affinities (they are able to form stable negative ions) and produce ion molecule adducts with gas phase nucleophiles such as Cl^-. Therefore, the response factors for the compound classes mentioned above were determined by both methane NICI (formation of negative ions by electron capture of thermal electrons) and hydroxyl ion NICI (negative ions are produced both by electron capture of electrons and by reactions with the gas phase nucleophil OH^-). Afterwards the response ratios between the different NICI techniques and conventional EI mass spectrometry were determined and compared with available biological activity data for the respective compounds.

2 EXPERIMENTAL

2.1 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

The instrumentation used for NICI mass spectrometry as well as details of the experimental conditions are described elsewhere (7,10,11). A brief summary is given in Table I. All chemicals and solvents were of analytical grade or higher. The gas chromatographic separations were carried out on a 30 m x 0.3 mm, i.d. fused silica capillary coated with 0.15 µm OV1 (Chrompack, Middelburg, The Netherlands). Separation conditions were as follows: injector temperature: 260 ^{0}C, carrier gas He at a flow velocity of 35 cm/s; injection of 1 µl sample splitless at 40 ^{0}C, after 2 min 40 to 130 ^{0}C at 30 ^{0}C/min and 130 to 270 ^{0}C at 5 ^{0}C/min.

Table 1: Step-by-step procedure for the determination of the NICI response of polar compounds extracted from air particulate matter.

1. High volume sampling using glass fiber filters of 142 mm (Gelman type 61635).

2. Soxhlet extraction with liquid CO_2 (12).

3. Prefractionation by HPLC of half the extract (ressolved in 1 ml CH_2Cl_2) on basic and acidic-buffered silica respectively (13,14). Acidic: 5 fractions, basic: 5 fractions (see (12)). 250x4.6 mm column, Lichrosorb Si-60-5 (E. Merck), Na_2HPO_4 pH 8.0 or $NaHSO_4$, pH 1.0. Gradient from Hexane to 60% CH_2Cl_2 at 20 min, then 100% CH_2Cl_2, flow rate 2 ml/min.

4. High resolution gas chromatography on OV 1 (fused silica capillary 30 m x 0.3 mm i.d.).

5. Detection by electron impact mass spectrometry at 70 eV or CH_4-NICI mass spectrometry (0.4 torr source pressure, 200 ^{0}C source temperature, 95 eV electron energy) or OH^--NICI mass spectrometry (0.15 torr CH_4 + 0.25 torr N_2O source pressure, 105 eV electron energy, 200 ^{0}C source temperature) on Hewlett-Packard 5985B/87A mass spectrometer (see also (10)).

Table 2: Identified compounds found in the most polar basic (B4, B5) and acidic fractions (A4, A5). Compounds with NICI response are marked. Mutagenic properties are indicated by M (mutagenic), MG (belonging to a mutagenic group) and O (non-mutagenic). Information about mutagenic properties is given in 15,16,17,18).

Fraction:

No.	Compound	Mol. weight	Found in A5	Found in B5	NICI response CH_4	NICI response OH^-	Mutagenic properties
1	Quinoline	129	-	+	-	+	M
3	Isoquinoline	129	-	+	-	+	O
4	2-methylquinoline	143	-	+	-	+	M
5	Methyquinoline/isoquinoline	143	-	+	-	+	?
6	7-methylquinoline	143	-	+	-	+	M
7	3-methylquinoline	143	-	+	-	+	M
8	2,6-+2,7-dimethylquinoline	157	-	+	-	+	?,MG
9	2,4-dimethylquinoline	157	-	+	-	+	?,MG
10	Dimethylquinoline/isoquinoline	157	-	+	-	+	?
11	N-methyltetrahydroisoquinoline	147	+	+	+	+	?
12	Ethylquinoline*	157	-	+	-	+	?,MG
13	Dimethylquinoline/isoquinoline	157	-	+	-	+	?
14	Trimethylquinoline*	171	-	+	-	+	?
15	Trimethylquinoline*	171	-	+	-	+	?
16	Trimethylquinoline*	171	-	+	-	+	?
17	N-phenylbenzeneamine	169	-	+	-	+	M
18	4-azafluorene	167	-	+	-	+	?,MG
19	Aromatic, unknown	183	-	+	-	+	?
20	Acridine	179	-	+	+	+	M
21	Phenanthridine + Benzo(f)quinoline	179	-	+	+	+	M
22	Benzoquinoline*	179	-	+	-	+	?,MG
23	Methylbenzoquinoline*	193	-	+	-	+	?
24	Dihydrodimethylacridine	209	-	+	-	+	?
25	Methylbenzoquinoline*	193	-	+	-	+	?,MG
26	Methylbenzoquinoline	193	-	+	-	+	?,MG
27	Hexadecanoic acid methylester	270	+	+	-	-	O
28	Dibutylphthalate	278	+	+	-	-	O(?)
29	Azadimethylphenanthrene*	207	-	+	-	-	?,MG
30	Azadimethylphenanthrene*	207	-	+	-	-	?,MG
31	Indeno(1,2,3-i,j)isoquinoline	203	-	+	+	+	?(M)
32	Azadimethylphenanthrene*	207	-	+	-	-	?,MG
33	Acenaphtho(1,2-b)pyridine	203	-	+	+	+	M
34	Benzo(lmn)phenanthridine	203	-	+	+	+	M
35	Aza-PAH, mixture	203+217	-	+	+	+	?;MG
36	Aza-PAH?	217	-	+	(+)	+	?
37	Aza-PAH?	217	-	+	-	+	?
38	Hexadecanoic acid butylester	312	+	+	-	-	O
39	Unknown	252(?)	-	+	-	-	?
40	Unknown	233	-	+	-	-	?
41	Octadecenamide	281	-	+	-	-	O(?)
42	Benzo(a)acridine	229	-	+	+	+	M
43	Aza-PAH	229	-	+	(+)	+	?,MG
44	Octadecenoic acid butylester	340	+	+	-	-	O
45	Aza-PAH	253	-	+	-	+	?,MG
46	Aliphatic amide	337	-	+	-	(+)	?,(O)

Table II continued

No.	Compound	Mol. weight	Found in A4	Found in B4	NICI response CH_4	NICI response OH^-	Mutagenic properties
47	Methylquinoline*	143	-	+	-	+	?
48	Dimethylquinoline	157	-	+	-	+	?
49	Phenylpyridine	155	-	+	-	+	?
50	Mixture	?	+	+	-	+	?
51	Acidic, N-containing compound	169	+	-	-	+	?
52	9H-Fluorenone	180	+	+	+	+	?,MG
53	Benzoquinoline*	179	-	+	-	+	?,MG
54	Methylfluorenone	194	+	+	+	+	?,MG
55	9H-xanthen-9-one	196	+	+	+	+	?,MG
56	Unknown	193	-	+	-	-	?
57	Methylfluorenone	194	+	+	+	+	?,MG
58	Benzo(c)cinnoline	180	-	+	-	-	?
59	Phenanthrenone*	194	+	+	+	+	?,MG
60	$C_{16}H_{13}NO$ or $C_{14}H_{11}N$	193	-	+	-	-	?
61	"	193	-	+	-	+	?
62	9,10-dihydro-9,9'-dimethyl-acridine*	209	-	+	-	+	?
63	9,10-Anthracenedione	208	+	+	+	+	?,MG
64	Dibutylphthalate	278	+	+	-	-	O(?)
65	Acidic compound	198	+	-	-	-	?
66	CN-PAH	205	-	+	-	-	?
67	Indeno(1,2,3-de)naphthridine	204	-	+	+	+	?,MG
68	Aza-PAH?	223	-	+	+	+	?,MG
69	Unknown	237	+	+	+	+	?
70	$C_{15}H_{10}O_2$ (aromatic)	222	+	+	-	+	?
	$C_{15}H_{11}N$ (aromatic)	205	-	+	+	+	?
71	$C_{15}H_{11}O_2$ (aromatic)	222	+	+	+	+	?
72	Diphenylpyrazole	220	-	+	-	-	?
73	Aza-PAH?	217	-	+	-	-	?
74	Unknown	220	+	+	+	+	?
75	Hexadecanoic acid butylester	312	+	(+)	-	-	O
76	Unknown	270	+	(+)	-	-	?
77	11H-benzo(a)fluoren-11-one	230	+	+	+	+	?,MG
78	7H-benzo(c)fluoren-7-one	230	+	+	+	+	?,MG
79	No Aza-PAH	229	-	+	-	(+)	?
80	11H-benzo(b)fluoren-11-one	230	+	+	+	+	?,MG
81	Octadecenoic acid butylester	340	+	+	-	-	O
82	Unknown	270	+	-	-	-	
83	Bis(2-ethylhexyl)-phthalate	390	+	(+)	-	-	O(?)
84	Carboxylic acid of PAH m.w. 202	248	+	-	-	-	?
85	Aza-PAH	253	-	+	+	+	?,MG
86	11H-benzo(be)aceanthrylen-11-one	254	+	+	+	+	?,MG
87	4H-cyclopenta(def) triphenylen-4-one	254	+	+	+	+	?,MG
88	Aza-PAH	253	-	+	+	+	?,MG
89	Silicone	-	-	+	-	-	O
90	Aza-PAH	253	-	+	+	+	?,MG
91	6H-benzo(cd)pyren-6-one	254	+	+	+	+	?,MG
92	Aliphatic amide	337	-	+	-	(+)	O
93	Aza-PAH	269	-	+	+	+	?,MG
94	Unknown	396	+	-	-	-	?
95	Keto-PAH	280	+	+	+	+	?

*: Other isomer possible

2.2 SAMPLING AND CLEAN-UP OF AIR PARTICULATE MATTER

Aerosols from indoor air (30-300 m^3) of an aluminium smelter and a coke-oven plant were collected on precleaned glass fiber filters of 142 mm diameter (Gelman Type 61635, Ann Arbor, MI, USA). Samples were liquid CO_2-extracted (12) for 8 hours. The residue was dissolved in 1 ml of methylene chloride and divided into two aliquots. The sample was separated further into different polarity fractions by high performance liquid chromatography (HPLC) on a silica column pretreated with either a basic or acidic salt (13). One aliquot was fractionated into 5 polarity ranges on the basic and one aliquot on the acidic silica surface. The same equipment and experimental conditions as described earlier (12) were used (see also Table I). Due to the reduced retention of basic polar compounds on the basic silica surface a solvent gradient to 100% CH_2Cl_2 was sufficient for complete elution. The same was valid for acidic compounds on acidic silica. Two fractions containing polar neutral to basic compounds were collected from the basic silica column and correspondingly from the acidic column (polar neutral to acidic) for further investigations.

3 RESULTS AND DISCUSSION

Extracts from indoor air samples taken in an aluminium smelter hall were chosen for the presented study due to following reasons:

- the more polar fractions are a complex mixture of different compound groups with large variations concerning mutagenic and/or carcinogenic properties
- the mutagenicity of many substances found in these extracts is at least partly documented.

To study the claimed correlation between biological activity and the ability of a compound to form stable negative ions the following detection methods were used:

1. Resonance capture NICI mass spectrometry employing CH_4 as reagent gas. This techniques allows to detect compounds which are able to form stable negative ions by pure electron capture processes.

2. Hydroxyl anion NICI mass spectrometry using CH_4/N_2O mixtures. This approach allows to test the statement of Horning et al. (5) which claimed that both a high electron affinity and reaction with oxygen (formation of a neutral radical and a stable negative ion) are necessary characteristics of a toxic compound. Dougherty et al. (9) found in addition that most toxic compounds react with gas phase nucleophiles such as Cl^-, O_2^- etc. OH^- behaves very similar to O_2^- (about same proton affinity) but is less corrosive to the ion source filament and was therefore chosen as gas phase nucleophile.

The air extracts were divided into two parts and prefractionated by HPLC on silica pretreated with either an acidic or basic salt to learn more about the acidic/basic properties of the compounds and to minimize interferences between acidic and basic substance classes. Table II summarizes the identified compounds in the most polar fractions 4 and 5. Additional information is given about their mutagenic properties and the possibility to detect them by NICI. Most of the compounds were either basic or approximately neutral (found in both acidic and basic fractions). Derivatization of all fractions with diazomethane (14) did not increase the number of detectable compounds considerably. Figure 1 and 2 compare the total ion current chromatograms for the basic fraction 4 and 5 obtained by electron impact ionization, CH_4-NICI and OH^--NICI. As can be seen most of the compounds detectable by CH_4-NICI are aza-arenes and keto-PAH. Many aza-arenes are mutagenic (see Tables) but only those with at least 3 rings were detected by OH_4-NICI. Non-mutagenic compounds such as fatty acids, phthalates, silicones and aliphatic amides did not give any response (see also Table III). Only little is known about the mutagenic properties of keto-PAH, but recently mutagenic effects of 2 to 5 ring quinones were reported using the Salmonella TA 104 tester strain (17). Furthermore, keto-PAH can undergo one-electron reduction to the semiquinone radical which in the presence of oxygen is regenerated to the original quinone producing the superoxide radical O_2^-. This redox cycling of quinones may lead to oxidative stress conditions (19). OH^--NICI allowed to detect all mutagenic aza-areanes including quinolines and all keto-PAH.

Table 3: NICI/EI response factor ratios for some selected compounds. Average values of three parallels are given. Standard deviations were in the order of 10-15%.

No	Compound	CH_4-NICI/EI	OH^--NICI/EI	Mutagenicity
1	Quinoline	<0.01	0.23	+
3	Isoquinoline	<0.01	0.09	-
4	2-methylquinoline	<0.01	0.24	+
6	7-methylquinoline	<0.01	0.14	+
7	3-methylquinoline	<0.01	0.24	+
8	2,6-+2,7-dimethyl quinoline	<0.01	0.22	?
17	N-phenylbenzeneamine	<0.01	0.29	+
18	4-azafluorene	<0.01	0.32	?
20	Acridine	0.02	0.33	+
21	Phenanthridine + benzo(f)quinoline	0.02	0.34	+
27	Hexadecanoic acid methylester	<0.01	<0.01	-
28	Dibutylphthalate	<0.01	<0.01	-,?
31	Indeno(1,2,3-i,j) isoquinoline	0.12	0.52	?
33	Acenaphtho(1,2-6) pyridine	0.63	2.14	+
34	Benzo(lmn)phenanthridine	0.22	0.71	+
38	Hexadecanoic acid butylester	<0.01	<0.01	-
41	Octadecenamide	<0.01	<0.01	-
42	Benzo(a)acridine	0.29	1.29	+
43	Aza-PAH m.w. 229	<0.01	0.16	?
44	Octadecenoic acid butylester	<0.01	<0.01	-
46	Aliphatic amide	<0.01	<0.01	?(0)
52	9H-fluorenone	1.41	4.2	?
63	9,10-anthracenedione	0.52	1.85	?
72	Diphenylpyrazol	<0.01	<0.01	?
77	11H-benzo(a)fluoren-11-one	0.37	1.60	?
78	7H-benzo(c)fluoren-7-one	0.33	1.17	?
80	11H-benzo(b)fluoren-11-one	0.36	1.48	?
81	Octadecenoic acid butylester	0.29	<0.01	0
83	Bis(2-ethylhexyl)-phthalate	<0.01	<0.01	?(0)
85	Aza-PAH m.w. 253	0.29	0.96	?
86	11H-benzo(bc) acenaphthrylen-11-one	0.19	0.76	?
91	6H-benzo(cd)pyren-6-one	0.30	1.00	?
92	aliphatic amide	<0.01	<0.01	0
	all aliphatic hydrocarbons (200^0C source temp.)	<0.01	<0.01	0
	all silicones	<0.01	<0.01	0

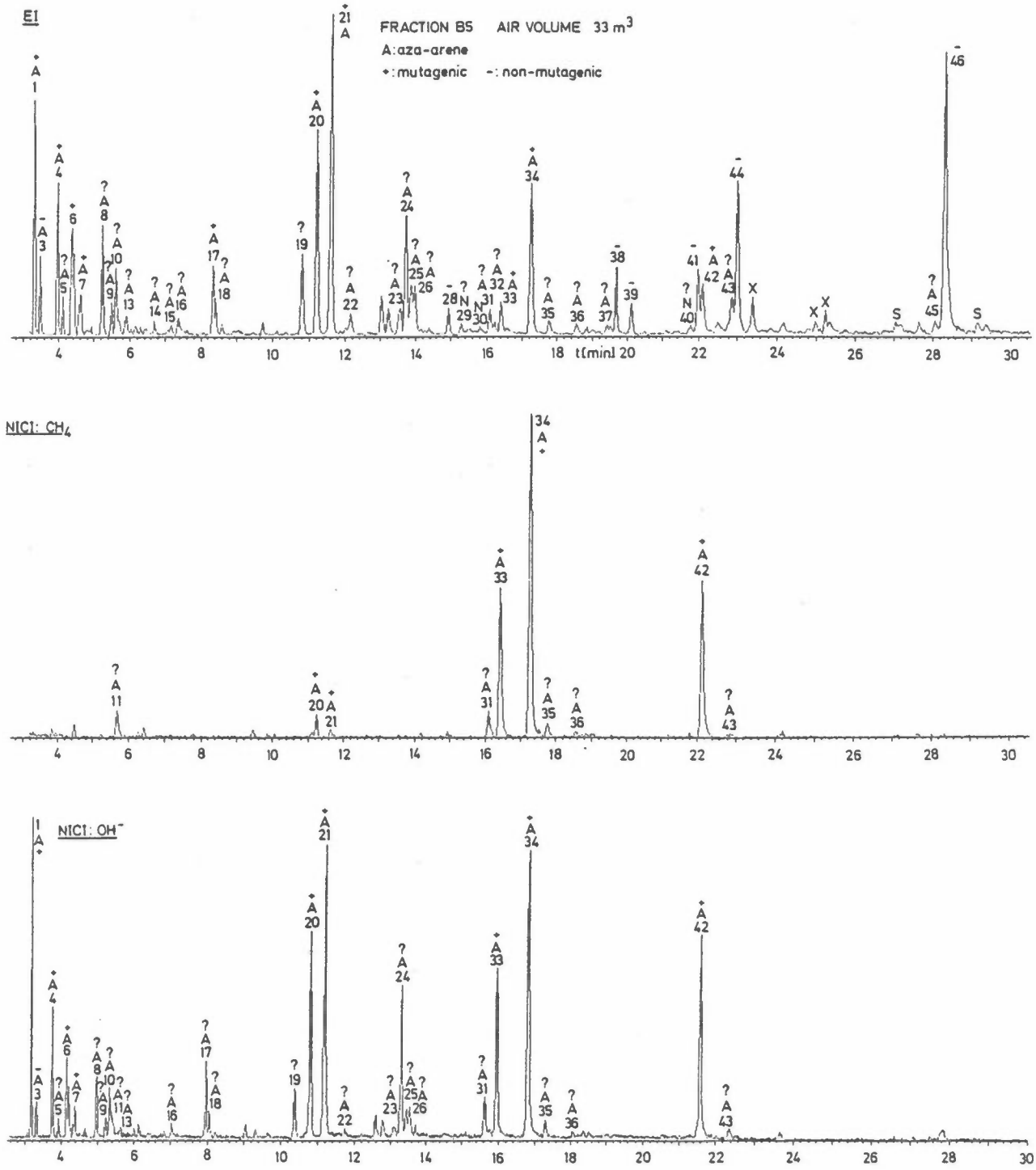

Figure 1: Comparison of the total ion chromatograms of fraction 5 recorded by EI, CH_4-NICI and OH^--NICI. For compound identification, see Table II.

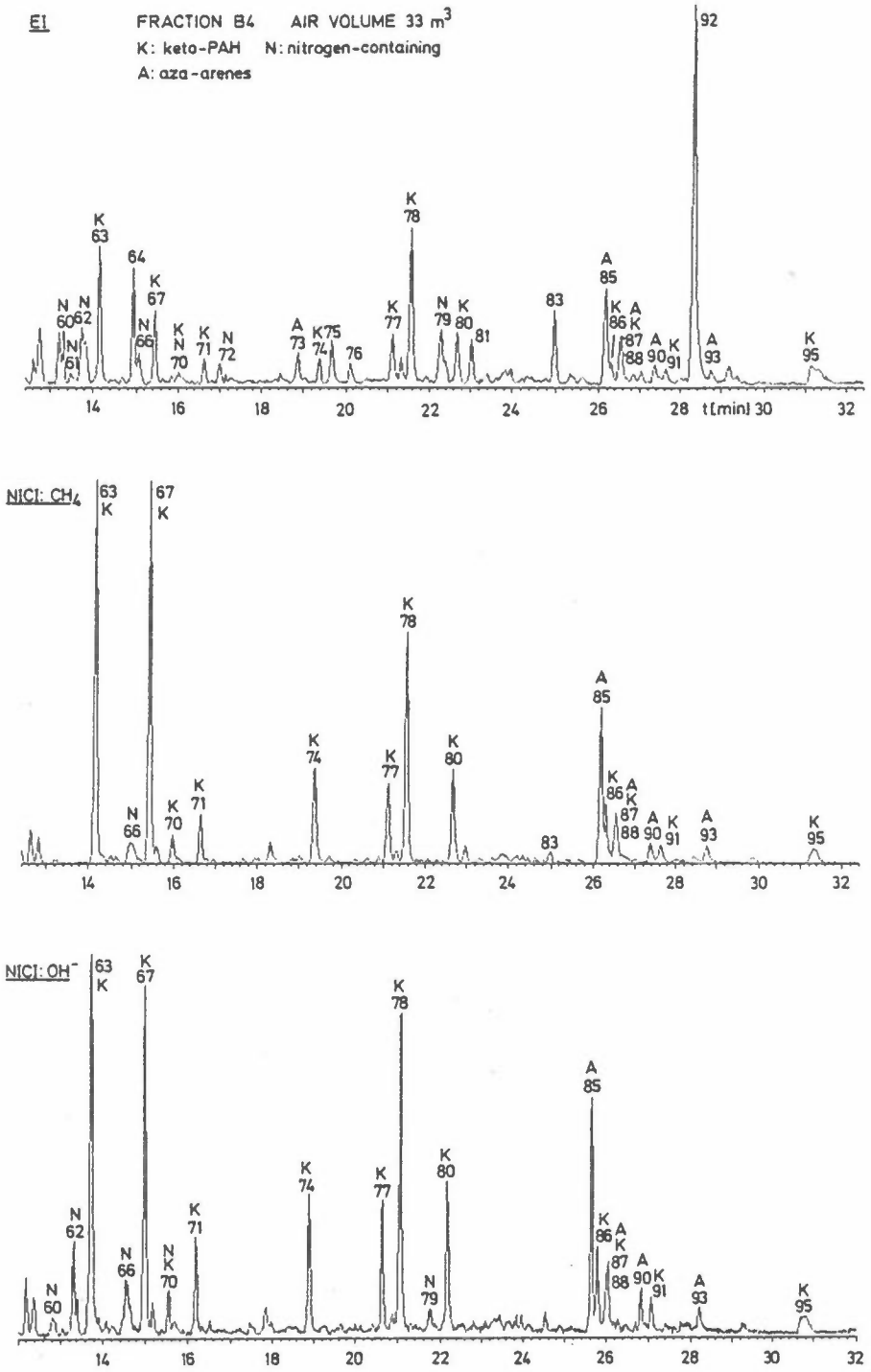

Figure 2. Comparison of the total ion chromatograms of fraction 4. Compound identification is given in Table II.

Non-mutagenic compounds such as fatty acids and their methyl esters, phtalates, aliphatic amide etc. were still not detectable. The following conclusions can be drawn:

- CH_4-NICI is a helpful additional detection technique to identify some mutagenic aza-arenes and all keto-PAH. Mutagenic 2-3 ring aza-arenes have low response factors. Other nonmutagenic compounds groups do not interfere.

- OH^--NICI allows to detect all aza-arenes and keto-PAH. Most of the mutagenic aza-arenes have OH^--NICI/EI response ratios > 0.2-1.3. The value for the non mutagenic isoquinoline is below this range. However, no further conclusions are possible since for many compounds no mutagenic data are available. The same is valid for keto-PAH (OH^--NICI/EI response ratio range > 0.8-4.2). The selectivity against non-mutagenic compounds (response ratio range 0.01-0.1) is still sufficient. The OH^--NICI response factors for phthalates and hydrocarbons are highly temperature-dependent and an ion-source temperature of 200^0C is recommended to maintain the selectivity shown in Table III.

- The presented work indicates further that NICI mass spectrometry is a useful technique which detects preferably compounds with at least mutagenic properties. However, more work has to be done (especially testing of the mutagenic properties of reference compounds) before final conclusions can be made concerning the relationship NICI-response/biological activity. OH^-NICI seems to be more suitable to identify compounds with biological activity since also substances, which react with gas phase nucleophiles, are detected.

Finally it was tried to compare the mutagenic activity of all four extracts (B4, B5, S4, S5) with the total amount of compounds detected by both NICI techniques. Single mutagenic azaarene compound concentrations were in the order of 100-1200 ng/m^3 (total air volume 33 m^3). Keto-PAH amounts were in the same order. The Salmonella test strain TA 98 and TA 100 were used with and without metabolic activation.

However, all samples had inhibiting effects to the bacterial growth and were partly toxic. Therefore, only small sample amounts could be applied for the test. Only fraction B4 showed some mutagenic activity (~77 revertants/m^3). All other samples were either non-mutagenic or the mutagenicity was covered by inhibiting effects. A further comparison with NICI results was therefore not possible. In opposite to the mutagenicity test, NICI was able to detect most mutagenic compounds in all fractions.

4 ACKNOWLEDGEMENT

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TITTEL
Negative ion chemical ionization mass spectrometry - a useful technique for the selective detection of polar substituted polycyclic aromatic hydrocarbons with mutagenic properties.

PROSJEKTLEDER
M. Oehme

NILU PROSJEKT NR.
N-8367

FORFATTER(E)
M. Oehme

TILGJENGELIGHET*
A

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3 STIKKORD (à maks. 20 anslag)
substituerte PAH | mutagenitet | analyse

REFERAT (maks. 300 anslag, 7 linjer).
Tidligere undersøkelser har vist at mange komponenter med toksiske egenskaper danner stabile negative ioner. Negativ ion massespektrometri-responsen av substituert PAH fra aluminiumindustrien ble bestemt og sammenlignet med mutagenitetsdata. Resultatene viser at den overfor nevnte sammenheng også gjelder for slike komponenter.

TITLE

ABSTRACT Earlier studies have shown that many compounds with toxic properties are able to form stable negative ions. The negative ion mass spectrometric response of polar substances found in indoor air extracts from aluminium smelters was determined and compared with available mutagenicity data. The results indicate that the relationship mentioned above also is valid for polar compounds.

*Kategorier: Åpen - kan bestilles fra NILU A
Må bestilles gjennom oppdragsgiver B
Kan ikke utleveres C