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## Nitrobenzene – method for the determination of nitrobenzene in workplace air using gas chromatography after thermodesorption

### Air Monitoring Method – Translation of the German version from 2018

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# Nitrobenzene – method for the determination of nitrobenzene in workplace air using gas chromatography after thermal desorption

## Air monitoring methods

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## Abstract

This analytical method is a validated measurement procedure for the determination of nitrobenzene [98-95-3] in workplace air in a concentration range of one tenth up to twice the currently valid OEL or MAK value of 0.51 mg/m<sup>3</sup>. With this method simultaneously airborne nitrobenzene in the gaseous state as well as particles are collected. Sampling is performed by drawing a defined volume of air through a quartz fibre filter located in the sampling head GGP-Mini with an adsorption tube filled with Tenax TA connected downstream using a suitable pump. The flow rate is set to 0.066 L/min with a recommended air sample volume of approx. 4 litres. The collected nitrobenzene is thermally desorbed and then analysed by means of gas chromatography using two detectors, a FID for quantification and a MSD to recognise potential interferences. The quantitative determination is based on a calibration function obtained by means of a multi-point calibration. The limit of quantification is 0.0085 mg/m<sup>3</sup> based on an air sample of 4 litres.

## Keywords

nitrobenzene; workplace measurement; hazardous substances; air analysis; workplace monitoring; glass fibre filter; Tenax TA; gas chromatography; GC-FID; GC-MSD; thermal desorption; GGP-Mini

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# Nitrobenzene – method for the determination of nitrobenzene in workplace air using gas chromatography after thermal desorption

<b>Method number</b>	1
<b>Application</b>	Air analysis
<b>Analytical principle</b>	Gas chromatography (thermal desorption)
<b>Completed in</b>	March 2018

## Summary

The analytical method described here enables the determination of nitrobenzene in workplace air from a tenth up to twice the currently valid OEL or MAK value of 0.51 mg/m<sup>3</sup> (0.1 ppm) [1, 2]. Nitrobenzene in the gaseous and particulate state can be simultaneously determined with this method. Sampling is performed using a suitable sampling pump to draw a defined volume of air through an adsorption tube filled with Tenax TA®, which has a GGP-Mini type sampling head fitted with a filter connected upstream to capture the aerosol fraction.

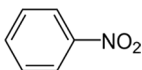
The analysis is carried out by means of gas chromatography with a flame ionisation detector (FID) after thermal desorption. At the same time a mass selective detector (MSD) is used, which can be useful for identification and quantification in the case of chromatographic interferences. A multiple-point calibration with calibration standards of known concentration is carried out for quantitative evaluation. There is a linear relationship between the peak area and the concentration.

## Characteristics of the method

Precision:	Standard deviation (rel.):	$s = 1.6\text{--}5.5\%$
	Expanded uncertainty:	$U = 21\%$
	in the concentration range of the limit of quantification up to twice the limit value and $n = 6$ determinations	
Limit of quantification:	0.0085 mg/m <sup>3</sup> for an air sample volume of 4 L	
Recovery:	$\eta = 1,0$ (100%)	
Sampling recommendations:	Sampling period:	60 min
	Air sample volume:	4 L
	Flow rate:	4 L/h

## Description of the substances

### Nitrobenzene [98-95-3]



Synonyms: mononitrobenzene, mirbane oil, nitrobenzol

Nitrobenzene is a colourless or occasionally due to impurities a pale-yellow liquid and has an odour similar to that of bitter almonds. Nitrobenzene has a high refractive index. Under standard conditions it has a density of 1.19867 g/cm<sup>3</sup>, melts at 5.7 °C and boils at 210.85 °C and the flash point is at 88 °C. Only traces of nitrobenzene are soluble in water, however, it is readily miscible with alcohols, ether and benzene. Nitrobenzene does not dissolve well in diluted sulphuric acid, however, it dissolves completely in concentrations of 80% and above. Solubility is only slightly temperature dependent.

Nitrobenzene is an important intermediary product used on a large scale for the production of various chemicals, such as aniline, benzidine, dinitrobenzene, trinitrobenzene, nitrobenzenesulfonic acid, fuchsine or quinoline. It is also used as a solvent, a component of lubricants, as a chemical reagent and as an additive for explosives. Additionally, it is used as an ignition-enhancing additive for diesel fuels.

The OEL and MAK value for nitrobenzene is 0.51 mg/m<sup>3</sup> (1 ppm) [1, 2]. The short-term exposure limit is classified in Peak Limitation Category II with an excursion factor of 4. Furthermore, the following footnote applies to nitrobenzene: "*may occur simultaneously as vapour and aerosol*". Detailed information on the toxicity of nitrobenzene can be found in the toxicological-occupational health documentation of MAK values [3].

$$1 \text{ mL/m}^3 (\text{ppm}) \triangleq 5.108 \text{ mg/m}^3$$

$$1 \text{ mg/m}^3 \triangleq 0.195 \text{ mL/m}^3 (\text{ppm})$$

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## 1 General principles

The analytical method described here enables the determination of nitrobenzene in workplace air from a tenth up to twice the currently valid OEL or MAK value of  $0.51 \text{ mg/m}^3$  (0.1 ppm) [1, 2]. Nitrobenzene occurring in the gaseous and particulate state can be simultaneously determined with this method. Sampling is carried out using a suitable sampling pump to draw a defined volume of air through a sampling system consisting of GGP-Mini type sampling head fitted with a quartz fibre filter and an adsorption tube filled with Tenax TA<sup>®</sup> connected downstream. Nitrobenzene occurring in a particulate state (free or bound) is thus deposited onto the filter and gaseous nitrobenzene is adsorbed onto the Tenax TA<sup>®</sup>. Deposited nitrobenzene particles that evaporate from the filter during sampling are collected downstream in the tenax tube.

After thermal desorption, nitrobenzene is determined by gas chromatography with a flame ionization detector (FID). At the same time a mass selective detector (MSD) is used, which can be useful for identification and quantification in the case of chromatographic interferences. A multiple-point calibration with calibration standards of known concentration is carried out for quantitative evaluation. There is a linear relationship between the peak area and the concentration.

## 2 Equipment, chemicals and solutions

### 2.1 Equipment

- Pump, suitable for a flow rate of 66 mL/min (e.g. Pocket Pump, from Analyt-MTC Messtechnik GmbH, 79379 Müllheim, Germany)
- Aerosol monitor for collecting the inhalable aerosols, e.g. GGP-Mini type sampling head with intake cone for 0.066 L/min (e.g. from Analyt-MTC Messtechnik GmbH)
- Quartz fibre filter, Munktell MK 360, Ø = 37 mm (e.g. from Binzer & Munktell Filter GmbH, 35088 Battenberg, Germany)
- Filter punch, Ø = 13 mm
- Muffle furnace
- Adsorption tubes made of stainless steel (6.3 mm x 90 mm, inner diameter of 5 mm), (e.g. from PerkinElmer LAS, 63110 Rodgau, Germany)
- Gauze loading rig (e.g. from PerkinElmer LAS, Order No. L4070023)
- Metal sieve for stainless steel tubes (e.g. from PerkinElmer LAS, Order No. L4071034)
- Retaining spring for metal packing gauze (e.g. from PerkinElmer LAS, Order No. L4071123)
- Gas chromatograph with thermal desorber, flame ionisation detector (FID), mass selective detector (MSD) and evaluation system
- Sealing caps (e.g. Swagelok with PTFE seals, PTFE)
- Capillary column e.g. DB-624: 30 m, film thickness of 1.4 µm; inner diameter of 0.25 mm, (e.g. from Agilent, 76337 Waldbronn, Germany)
- Gas meter or stopwatch and soap bubble flowmeter
- Analytical balance
- Volumetric flasks, nominal volume 100 mL
- Positive displacement pipette, Microman type, 1 to 10 µL, (e.g. from Gilson, 65555 Limburg, Germany)
- Tweezers

### 2.2 Chemicals

- Nitrobenzene, p.a., purity ≥ 99%, (e.g. from Merck, 64293 Darmstadt, Germany)
- Methanol, p.a., purity ≥ 99.5%, (e.g. from Merck, 64293 Darmstadt, Germany)
- Tenax TA® (35–60 mesh), (e.g. from Agilent Technologies, 64289 Darmstadt, Germany)

#### Gases for operation of the gas chromatograph/thermal desorber

- Helium 5.0 (carrier gas)
- Purified or synthetic air (free of hydrocarbons), dew point better than –40 °C
- Hydrogen 5.0
- Nitrogen 5.0

### 2.3 Preparation of the sampling system

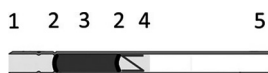
The sampling system – consisting of a filter and an adsorption tube connected downstream – is prepared as follows before use:

Adsorption tubes filled with Tenax TA® (75 mg Tenax TA® 35–60 mesh) are not commercially available and must be prepared and conditioned in the laboratory. The quartz fibre filters are conditioned in the muffle furnace at 500 °C for four hours prior to sampling.

#### 2.3.1 Adsorption tubes

Adsorption tubes made of stainless steel are filled with 75 mg Tenax TA® (35–60 mesh) and the adsorbent is slightly compressed by tapping. It is important to ensure that the adsorbent is not compressed too much. The filled tubes are fitted into the gauze loading rig and metal packing gauze is carefully pushed to the end of the adsorbent layer. Then a spring is pushed up to the gauze in order to prevent the gauze falling out of the tube (see Figure 1). The flow resistance must be checked before an adsorption tube is used for the first time. This should not exceed 30 hPa at a flow rate of 1 L/min.

Before their first use, the adsorption tubes filled with Tenax TA® are conditioned for approx. 20 minutes in the thermal desorber at 300 °C and then tested for blank values. Then they are sealed with suitable caps for storage. The tubes can be re-used after analysis is complete.



**Figure 1** Schematic illustration of the adsorption tubes used

- |                                     |                       |
|-------------------------------------|-----------------------|
| 1 Connection to the pump            | 4 Spring for fixation |
| 2 Retention gauze for the adsorbent | 5 Sampling opening    |
| 3 Adsorbent Tenax TA®               |                       |

#### 2.3.2 Quartz fibre filters

Before their use, the quartz fibre filters are conditioned in the muffle furnace for four hours at 500 °C. This preparatory step reduces the background of thermally desorbable compounds to a minimum.

### 2.4 Solutions

Stock solution: Nitrobenzene (1.20 mg/mL)

0.1 mL of nitrobenzene is pipetted into a 100 mL volumetric flask and weighed. The volumetric flask is then filled to the mark with methanol and shaken.

### Calibration solutions:

The calibration solutions are prepared by diluting the stock solution with methanol in the ratio of 1:10 (Calibration Solution I) or 1:100 (Calibration Solution II) (Table 1).

The prepared solutions can be stored in the refrigerator at approx. 4 °C for at least 6 months. The date of preparation must be noted on the volumetric flask.

**Table 1** Concentration of the stock solution and calibration solutions

Substance	Stock solution	Calibration solution I	Calibration solution II
	[g/L]	[µg/µL]	[µg/µL]
Nitrobenzene	1.20	0.120	0.0120

## 2.5 Calibration standards

For the purpose of calibration, adsorption tubes filled with Tenax TA® are spiked with aliquots of 1 to 10 µL of the calibration solutions (see Table 1). Clean air or nitrogen is then drawn through the adsorption tubes at a flow rate of 30 mL/min for 10 minutes in order to remove the excess methanol solvent. The spiked adsorption tubes contain the calibration masses shown in Table 2.

**Table 2** Content of nitrobenzene in then calibration samples

Solution	Dosing volume	Spiked mass	Concentration at an air sample volume of 4 L
	[µL]	[µg]	[mg/m³]
Calibration solution II	1	0.0120	0.003
	5	0.060	0.015
	10	0.120	0.030
Calibration solution I	2.5	0.300	0.075
	5	0.600	0.150
	7.5	0.900	0.225
	10	1.20	0.300
Stock solution	2.5	3.00	0.750
	5	6.00	1.50

## 3 Sampling and sample preparation

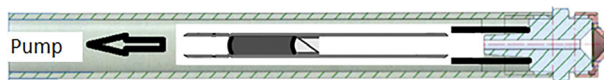
The GGP-Mini type sampling head is fitted with a prepared quartz fibre filter and an intake cone suitable for the flow rate of 0.066 L/min at the beginning of sampling. An adsorption tube filled with Tenax TA® is connected to the tube connections of the



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sampling head and the sampling pump [4]. The connection between the sampling head and the adsorption tube is established by using a short section of Viton® tube.

The definition of an inhalable dust is fulfilled by this sampling system [5, 6]. The schematic set-up of the sampling system is illustrated in Figure 2.



**Figure 2** Schematic illustration of the sampling system consisting of a GGP-Mini sampling head and an adsorption tube connected downstream

The pump and the sampling system are either worn by a person while performing their activities or stationary sampling is carried out. Air from the breathing zone is sampled. The opening of the adsorption tube should be freely accessible. An air sample volume of 4 litres is achieved, at a pre-selected flow rate of 0.066 L/min and a sampling time of 60 minutes. The important parameters for the determination of the concentration in air (sample volume, temperature, air pressure and relative humidity) are documented in the sampling record.

After sampling, the filter is removed from the sampling head, folded using tweezers and pushed into the end of the adsorption tube that faces towards the sampling head. Then the tube is sealed at both ends using Swagelok caps with PTFE seals until analysis.

## 4 Operating conditions for chromatography

Apparatus:	Clarus 600 gas chromatograph with flame ionisation detector (FID), Clarus 600T mass selective detector (MSD), PerkinElmer LAS	
Column:	Material:	Fused silica capillary
	Stationary phase:	DB-624 (6% cyanopropyl-phenylpolysiloxane and 94% dimethylpolysiloxane)
	Length:	30 m
	Inner diameter (ID):	0.25 mm
Eluate flow splitter:	Film thickness:	1.4 µm
	Graphpack-3D/2-eluate flow splitter, Order No. GC 08194-40, from Gerstel, Mülheim an der Ruhr, Germany	
	Split ratio:	1:1 (FID/MSD)
Detectors:	FID and MSD	
Detector temperature (FID):	320 °C	
Detector gases:	Hydrogen (45 mL/min), synthetic air (450 mL/min)	
Temperature program:	10 min at 35 °C, increased by 10 °C/min up to 240 °C (10 min)	

**MS operational conditions**

Temperatures:	Ion source:	180 °C
	Transfer line:	200 °C
Type of ionisation:	Electron impact (EI)	
Pressure of the ion source:	$3 \times 10^{-6}$ kPa	
Ionisation energy:	70 eV	
Mass range:	35–520 amu	

Under the conditions given here the retention time for nitrobenzene is 24.5 minutes (see Table 7 in the Appendix).

**5 Analytical determination**

The adsorption tubes are heated in the thermal desorber in the opposite direction to that of sampling. The nitrobenzene desorbed in this manner is transferred by means of a carrier gas into a cold trap packed with Tenax TA®. After complete desorption of the nitrobenzene, the cold trap is heated spontaneously, so that the analyte is transferred to the separation column as a narrow substance plug.

The thermal desorber is set to the following instrumental conditions:

**Conditions of the thermal desorption**

Apparatus:	Turbomatrix 650 (PerkinElmer LAS)
Desorption temperature:	280 °C
Desorption duration:	20 min
Valve temperature:	220 °C
Temperature of the transfer line:	200 °C
Transfer line:	1.5 m deactivated non-loaded pre-column, (ID 0.32 mm)
Cold trap (adsorption):	–30 °C
Cold trap (injection):	280 °C
Cold trap filling:	20 mg of Tenax TA®
Heating rate:	40 °C/s
Carrier gas:	Helium
Carrier gas flow:	1.7 mL/min
Split (before the cold trap):	200 mL/min (input split)
Flow rate through the cold trap:	10 mL/min (desorption flow)
Split (after the cold trap):	20 mL/min (output split)
Purge drying phase:	1 min at room temperature at 50 L/min

After the thermal desorber and gas chromatograph have been prepared, the calibration and analytical samples are measured. Should other thermal desorption devices be used, then the instrumental conditions must be adapted accordingly.

## 6 Calibration

The calibration samples prepared according to Section 2.5 are analysed as described in Sections 4 and 5 in order to obtain the calibration function. The peak areas obtained are plotted versus the corresponding spiked mass (see Table 2). The calibration function is linear in the investigated concentration range and should be regularly checked during routine analysis. For this purpose, a calibration standard of known concentration must be analysed in each analytical series.

## 7 Calculation of the analytical result

Based on the determined peak areas, the corresponding mass  $X$  in  $\mu\text{g}$  per sample is obtained from the respective calibration curve. The corresponding mass concentration ( $\rho$ ) is calculated according to Equation (1) below:

$$\rho = \frac{X}{V \times \eta} \quad (1)$$

Equation (2) below enables calculation of the value at 20 °C and 1013 hPa:

$$\rho_0 = \rho \times \frac{273+t_a}{293} \times \frac{1013}{p_a} \quad (2)$$

where:

- $\rho$  is the mass concentration of nitrobenzene in the ambient air in  $\text{mg}/\text{m}^3$  at  $t_a$  and  $p_a$
- $\rho_0$  is the mass concentration of nitrobenzene in  $\text{mg}/\text{m}^3$  at 20 °C and 1013 hPa
- $X$  is the mass of nitrobenzene in the analytical sample in  $\mu\text{g}$
- $V$  is the air sample volume (calculated from the flow rate and the sampling period) in L
- $\eta$  is the recovery
- $t_a$  is the temperature during sampling in °C
- $p_a$  is the atmospheric pressure during sampling in hPa

## 8 Reliability of the method

The characteristics of the method were calculated as stipulated in DIN EN 482 [7], DIN EN 1076 [8], DIN EN 13936 [5] and DIN 32645 [9]. The precision data and the influence of the humidity were determined in each case on the basis of a series of six sample measurements.

The samples were prepared by spiking the filters with solutions (see Section 2.4; Table 1). A spiked filter was then immediately fitted into the sampling head. After attaching the intake cone, the sampling head was connected to the adsorption tube and humidified air was drawn through the sampling system. After sampling, the filter is folded using tweezers and pushed from the rear side into the adsorption tube. The sample is then analysed according to Sections 4 and 5. Storage stability was determined by direct spiking onto the adsorption tube.

### 8.1 Precision and expanded uncertainty

For the purpose of determining the precision, three experimental series with nitrobenzene concentrations in the range of one tenth to twice the MAK value were prepared. After spiking the filters and connecting a sampling head upstream of the adsorption tube, 4 litres of air with a relative humidity of 80% were drawn through the sampling system at room temperature (23 °C).

The expanded uncertainty was estimated as stipulated in DIN EN 482 [7] and calculated according to [10] taking all relevant influencing factors into consideration. The expanded uncertainty of the entire method consists principally of the sampling uncertainty contributions (e.g. air sample volume, deviation from the sampling convention) and the analytical preparation (scatter of the calibration function, fluctuations in the transfer as well as the reproducibility). The resulting characteristics, such as relative standard deviation and expanded uncertainty, are listed in Table 3.

**Table 3** Standard deviation (rel.), expanded uncertainty  $U$  and recovery for  $n = 6$  determinations

Spiked mass of nitrobenzene	Concentration of nitrobenzene	Standard deviation (rel.)	Expanded uncertainty $U$	Recovery
[ $\mu\text{g}$ ]	[ $\text{mg}/\text{m}^3$ ]	[%]	[%]	[%]
0.24	0.060	5.5	21.3	99
2.4	0.60	1.7	20.8	100
4.8	1.20	1.6	20.8	100

### 8.2 Recovery and influence of the air humidity

The recoveries were calculated using the precision experiments (see Section 8.1). The mean recovery was 100%.

### 8.3 Influence of the temperature

The influence of the temperature during sampling was determined by conducting two experimental series. After spiking the filter with 5  $\mu\text{L}$  of stock solution, equivalent to 6.0  $\mu\text{g}$  of nitrobenzene, and subsequent connection of the filter upstream of the adsorption tube four litres of air with a relative humidity of 50% were drawn through the sampling system at 10 °C and 40 °C. No influence from the temperature could be detected (see Table 4).

**Table 4** Standard deviation (rel.) and recovery for  $n = 3$  determinations

Spiked mass of nitrobenzene	Temperature	Concentration of nitrobenzene	Standard deviation (rel.)	Recovery
[ $\mu\text{g}$ ]	[ $^{\circ}\text{C}$ ]	[ $\text{mg}/\text{m}^3$ ]	[%]	[%]
6.0	10	1.5	0.75	100
6.0	40	1.5	0.01	103

#### 8.4 Limit of quantification

The limit of quantification was calculated in the same manner as the calibration line method described in DIN 32645 [9] with a statistical certainty of  $P = 95\%$  und  $k = 3$ .

The limit of quantification was determined by spiking filters with aliquots of 1 to 10  $\mu\text{L}$  of calibration solution II (see Section 2.4; Table 1) and pushing the filter from the rear side into the end of the adsorption tube using tweezers. Nitrogen is then drawn through the adsorption tubes at a flow rate of 30  $\text{mL}/\text{min}$  for 10 minutes in order to remove the excess methanol. For this purpose, the rear ends of the adsorption tubes were connected to the nitrogen supply. According to the calibration line method ( $P = 95\%$ ,  $k = 3$ ) the limit of quantification of nitrobenzene is 0.0085  $\text{mg}/\text{m}^3$  (0.034  $\mu\text{g}$  absolute) based on an air sample volume of 4 litres.

#### 8.5 Capacity of the sampling system

The capacity of the sampling system is determined by spiking an adsorption tube with 5  $\mu\text{L}$  of the stock solution (see Section 2.4), which is equivalent to 6.0  $\mu\text{g}$  of nitrobenzene. A second adsorption tube was then connected downstream and 8 litres of air were drawn through the combined tubes at room temperature (23  $^{\circ}\text{C}$ ) and a relative humidity of 80%. No breakthrough was observed.

#### 8.6 Storage stability

Tests on storage stability of the loaded sampling systems were carried out over periods of two and four weeks. For this purpose, experimental series were prepared with 0.24  $\mu\text{g}$  and 4.8  $\mu\text{g}$  of nitrobenzene – equivalent to 0.060  $\text{mg}$  and 1.20  $\text{mg}$  of nitrobenzene per  $\text{m}^3$  at an air sample volume of 4 litres.

The samples were dosed by applying aliquots in the  $\mu\text{L}$  range directly onto the Tenax TA<sup>®</sup> adsorbent in the adsorption tubes and then four litres of air with a relative humidity of 80% were drawn through the tubes. The adsorption tubes were sealed with Swagelok caps and stored at room temperature.

After two as well as after four weeks three adsorption tubes were prepared and analysed according to Sections 4 and 5 in each case. The results are listed in Table 5. During the four-week period no losses could be detected, therefore storage stability over a period of four weeks is ensured.

**Table 5** Recoveries of nitrobenzene after a storage period of two and four weeks at room temperature.

Spiked mass of nitrobenzene [µg]	Detected mass [µg] after a storage period of	
	2 weeks	4 weeks
0.24	0.26	0.24
4.8	4.83	4.82

## 8.7 Interference

On account of the low specificity of flame ionisation detectors, interference is principally possible due to components with the same retention time. The results of the mass selective detection are used to confirm the analytical results.

## 9 Discussion

Nitrobenzene can be determined in workplace air in a concentration range of a tenth up to twice the currently valid OEL or MAK value of 0.51 mg/m<sup>3</sup> at an air sample volume of 4 L (0.004 m<sup>3</sup>) with the analytical method described here. Furthermore, the analytical method is suitable for monitoring compliance with the peak limit (short-term exposure limit).

The method described here was examined using two different concentrations. For this purpose, six sample carriers were each spiked with 0.60 µg and 1.20 µg of nitrobenzene in the laboratory of the developer of the method (LfU – State Environmental Agency Rhineland-Palatinate) and that of the examiner of the method (BASF SE Environmental Analysis). 4 litres of ambient air at an air humidity of approx. 55% were then drawn through the sample carriers. The sample carriers were sealed and exchanged between the laboratories, so that both laboratories each analysed three samples that had been spiked in-house and three spiked by the other laboratory. The analyses were carried out simultaneously in accordance with Sections 4 and 5 after five days. Recoveries of 91 to 98% were obtained. The exact results can be found in Table 6.

Sampling with the mini GGP sampling system ensures that the airborne aerosol fraction is always captured in its entirety [11].

**Table 6** Results of testing the measurement method for nitrobenzene

	Theoretical concentration	Laboratory 1 (LfU)		Laboratory 2 (BASF SE)	
		Concentra- tion detected	Recovery	Concentra- tion detected	Recovery
	[mg/m <sup>3</sup> ]	[mg/m <sup>3</sup> ]	[%]	[mg/m <sup>3</sup> ]	[%]
Experimental series 1	0.150	0.126	91	0.138	92
Experimental series 2	0.300	0.281	94	0.295	98

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## Appendix

**Table 7** Retention times of selected solvents (Separation column 30 m DB-624, for analytical conditions see Section 4)

Retention time [min]	Substance	CAS number
3.26	Methanol	67-56-1
4.48	Ethanol	64-17-5
5.22	Acetone	67-64-1
5.63	2-Propanol	67-63-0
6.03	Methyl acetate	79-20-9
6.66	<i>tert</i> -Butyl alcohol	75-65-0
7.86	<i>n</i> -Hexane	110-54-3
8.91	1-Propanol	71-23-8
10.49	2-Butanone	78-93-3
10.85	Ethyl acetate	141-78-6
11.27	Tetrahydrofuran	109-99-9
11.37	<i>sec</i> -Butyl alcohol	78-92-2
12.03	Cyclohexane	110-82-7
12.98	Isobutyl alcohol	78-83-1
13.26	Isopropyl acetate	108-21-4
13.64	<i>n</i> -Heptane	142-82-5
14.33	1-Propylene glycol 1-methyl ether	107-98-2
14.42	<i>n</i> -Butyl alcohol	71-36-3
14.69	Methylcyclohexane	108-87-2
15.26	Propyl acetate	109-60-4
16.46	4-Methyl-2-pentanone	108-10-1
16.72	Toluene	108-88-3
17.01	<i>n</i> -Octane	111-65-9
17.06	Isobutyl acetate	110-19-0
17.86	2-Hexanone	591-78-6
18.10	<i>n</i> -Butyl acetate	123-86-4
18.18	Cyclopentanone	120-92-3
18.92	Ethylene glycol monomethyl ether acetate	110-49-6
19.20	Ethylbenzene	100-41-4
19.38	m+p-Xylene	108-38-3; 106-42-3
19.46	<i>n</i> -Nonane	111-84-2



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**Tab. 7** (continued)

Retention time [min]	Substance	CAS number
19.51	Propylene glycol 1-methyl ether-2-acetate	108-65-6
19.98	<i>o</i> -Xylene	95-47-6
20.16	Ethylene glycol monoethyl ether acetate	111-15-9
20.33	Cyclohexanol	108-93-0
20.56	Cumene	98-82-8
20.61	Ethylene glycol monobutyl ether	111-76-2
20.67	Cyclohexanone	108-94-1
21.17	<i>n</i> -Propyl benzene	103-65-1
21.44	1,3,5-Trimethylbenzene	108-67-8
21.47	<i>n</i> -Decane	124-18-5
21.64	Diisobutyl ketone	108-83-8
21.99	1,2,4-Trimethylbenzene	95-63-6
22.62	1,2,3-Trimethylbenzene	526-73-8
23.58	Benzyl alcohol	100-51-6
23.61	Ethylene glycol monobutyl ether acetate	112-07-2
24.48	Nitrobenzene	98-95-3
25.20	Tetrahydronaphthalene	119-64-2
26.58	2-Phenoxyethanol	122-99-6