

**Joint Assessment of
Commodity Chemicals No. 36**

***n*-Butyl Methacrylate
Isobutyl Methacrylate**

CAS No. 97-88-1

CAS No. 97-86-9

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THE ECETOC SCHEME FOR THE JOINT ASSESSMENT OF COMMODITY CHEMICALS

This report has been produced as part of the ECETOC programme for preparing critical reviews of the toxicology and ecotoxicology of selected existing industrial chemicals.

In the programme, commodity chemicals, that is those produced in large tonnage by several companies and having widespread and multiple uses, are jointly reviewed by experts from a number of companies with knowledge of the chemical. It should be noted that in a JACC review only the chemical itself is considered; products in which it appears as an impurity are not normally taken into account.

ECETOC is not alone in producing such reviews. There are a number of organisations that have produced and are continuing to write reviews with the aim of ensuring that toxicological knowledge and other information are evaluated. Thus a producer, government official or consumer can be informed on the up-to-date position with regard to safety information and standards. Within ECETOC we do not aim to duplicate the activities of others. When it is considered that a review is needed every effort is made to discover whether an adequate review exists already; if this is the case the review is checked, its conclusions summarised and the literature published subsequent to the review assessed. To assist ourselves and others working in this field we have published a summary of international activities incorporating work planned, in hand, or completed on the review of safety data for commodity chemicals. Interested readers should refer to our Technical Report No. 71 entitled "Inventory of Critical Reviews on Chemicals".

This document presents a critical evaluation of the toxicology and ecotoxicology of the two isomers of butyl methacrylate, *n*-butyl methacrylate (CAS No. 97-88-1; *n*-BMA) and isobutyl methacrylate (CAS No. 97-86-9; *i*-BMA). The abbreviation *n*-BMA/*i*-BMA is used in this report whenever the text is applicable to both isomers.

The *n*-BMA and *i*-BMA isomers are reviewed in the same document because of the close similarity of their chemical structure, physical and chemical properties, environmental profiles and toxicity data. Furthermore the two esters are frequently produced in the same production plant and their use pattern is very similar. The decision to review both *n*-BMA and *i*-BMA together was based on the contention that there are no fundamental differences between the toxicity and environmental profiles of the alcoholic moieties of *n*-butanol and isobutanol (IPCS, 1987).

To compensate for the scarcity of data on some endpoints, available information on structurally analogous compounds and hydrolysis products is offered in Chapter 9. These data were employed in the hazard assessment of *n*-BMA/*i*-BMA.

***n*-Butyl Methacrylate (CAS No. 97-88-1) and Isobutyl Methacrylate (CAS No. 97-86-9)**

CONTENTS

1. SUMMARY AND CONCLUSIONS.....	1
2. IDENTITY, PHYSICAL AND CHEMICAL PROPERTIES, ANALYTICAL METHODS	4
2.1 IDENTITY	4
2.1.1 <i>n</i> -Butyl Methacrylate	4
2.1.2 Isobutyl Methacrylate	5
2.2 PHYSICAL AND CHEMICAL PROPERTIES.....	6
2.3 CONVERSION FACTORS	8
2.4 ANALYTICAL METHODS	9
2.4.1 Purity of <i>n</i> -BMA/ <i>i</i> -BMA	9
2.4.2 <i>n</i> -BMA/ <i>i</i> -BMA in Products	9
2.4.3 <i>n</i> -BMA/ <i>i</i> -BMA in Air	10
2.4.4 <i>n</i> -BMA/ <i>i</i> -BMA in Aqueous Solutions and Dispersions.....	11
2.4.5 Biological Media	11
3. PRODUCTION, STORAGE, TRANSPORT AND USE	13
3.1 PRODUCTION.....	13
3.2 STORAGE	13
3.3 TRANSPORT.....	13
3.4 USE	13
4. ENVIRONMENTAL DISTRIBUTION AND TRANSFORMATION.....	15
4.1 EMISSIONS	15
4.1.1 Natural sources.....	15
4.1.2 Emissions During Production and Use	15
4.2 ENVIRONMENTAL DISTRIBUTION	16
4.3 ENVIRONMENTAL FATE AND BIOTRANSFORMATION.....	17
4.3.1 Atmospheric Fate.....	17
4.3.2 Aquatic Fate.....	17
4.3.3 Terrestrial Fate.....	18
4.3.4 Biodegradation.....	18
4.3.5 Bioaccumulation.....	19
4.3.6 Evaluation	19

8.5 ENVIRONMENTAL LEVELS AND HUMAN EXPOSURE	21
5.1 ENVIRONMENTAL LEVELS	21
5.2 HUMAN EXPOSURE LEVELS AND HYGIENE STANDARDS	21
5.2.1 Non-occupational Exposure	21
5.2.2 Occupational Exposure	21
5.2.3 Hygiene Standards	23
6. EFFECTS ON ORGANISMS IN THE ENVIRONMENT	24
6.1 MICROORGANISMS	24
6.2 AQUATIC ORGANISMS	24
6.3 SUMMARY AND EVALUATION	26
7. KINETICS AND METABOLISM	27
7.1 BODY DISTRIBUTION	27
7.2 IN VITRO METABOLISM	27
7.2.1 Reaction with Glutathione	27
7.2.2 Hydrolysis Catalysed by Liver Enzymes	27
7.2.3 Other Studies	28
7.2.4 Summary	28
7.3 EVALUATION	29
8. EFFECTS ON EXPERIMENTAL ANIMALS AND IN VITRO TEST SYSTEMS	30
8.1 ACUTE TOXICITY	30
8.1.1 Oral	30
8.1.2 Dermal	31
8.1.3 Inhalation	31
8.1.4 Intraperitoneal	32
8.1.5 Other routes	33
8.1.6 Summary	33
8.2 SKIN, RESPIRATORY TRACT AND EYE IRRITATION, SENSITISATION	33
8.2.1 Skin Irritation	33
8.2.2 Eye Irritation	35
8.2.3 Respiratory Tract Irritation	36
8.2.4 Sensitisation	37
8.2.5 Evaluation	39
8.3 REPEATED DOSE TOXICITY	40
8.3.1 Summary	40
8.4 GENETIC TOXICOLOGY	41
8.4.1 <i>In Vitro</i> Bacterial Gene Mutation Assays	41
8.4.2 <i>In Vivo</i> Chromosome Damage Assays	42

42	8.4.3 Summary and Evaluation
42	8.5 CHRONIC TOXICITY AND CARCINOGENICITY
43	8.5.1 Evaluation
43	8.6 REPRODUCTIVE TOXICITY
43	8.6.1 Evaluation
45	9.1 METABOLISM
45	9.1.1 Hydrolysis
46	9.1.2 Metabolism of Hydrolysis Products
46	9.2 CHRONIC TOXICITY STUDIES
48	9.3 REPRODUCTIVE TOXICITY
48	9.3.1 Developmental Toxicity
49	9.3.2 Fertility and Effects on Reproductive Organs
50	9.3.3 Conclusion
51	10. EFFECTS ON HUMANS
51	10.1 ACUTE AND SUBCHRONIC TOXICITY
51	10.2 IRRITATION AND SENSITISATION
51	10.2.1 Skin Irritation and Sensitisation
51	10.2.2 Evaluation
52	10.3 HAZARD ASSESSMENT
53	11. FIRST AID AND SAFE HANDLING ADVICE
53	11.1 FIRST AID AND MEDICAL TREATMENT
53	11.1.1 Skin and Eye Injuries
53	11.1.2 Inhalation
53	11.1.3 Ingestion
53	11.2 SAFE HANDLING
53	11.2.1 Safety at Work
54	11.2.2 Storage Safety
54	11.2.3 Fire Safety and Extinguishants
54	11.2.4 Protection against Fire and Explosion
55	11.3 MANAGEMENT OF SPILLAGE AND WASTE
56	APPENDIX A. METABOLISM OF METHACRYLIC ACID, <i>n</i> -BUTANOL AND ISOBUTANOL
56	A.1 METHACRYLIC ACID
57	A.2 <i>n</i> -BUTANOL
58	A.3 ISOBUTANOL

BIBLIOGRAPHY59

REFERENCES NOT QUOTED69

MEMBERS OF THE TASK FORCE75

MEMBERS OF THE SCIENTIFIC COMMITTEE76

1. SUMMARY AND CONCLUSIONS

Because of the close similarity of their chemical structure, production methods and use pattern, the two isomers of butyl methacrylate, *n*-butyl methacrylate (*n*-BMA) and *i*-sobutyl methacrylate (*i*-BMA) are considered together in this report. The abbreviation *n*-BMA/*i*-BMA is used whenever the text is applicable to both isomers.

At room temperature, *n*-BMA/*i*-BMA is a clear, colourless, flammable liquid with a faint, characteristic ester odour. Both compounds have a low solubility in water and are soluble in most organic solvents.

In the EU, about 30 kt of *n*-BMA and 8 kt of *i*-BMA were produced in 1994. Environmental releases during production and major industrial uses are very low.

When released into the environment, the majority (95%) of *n*-BMA/*i*-BMA will partition into the atmosphere. The atmospheric half-life of *n*-BMA/*i*-BMA has been estimated to be between 5.6 and 7.5 hours depending on the parameters of the calculation. In water *n*-BMA/*i*-BMA is readily biodegradable. A moderate bioaccumulation potential is expected. A half-life of 13 hours for *n*-BMA and 5.6 hours for *i*-BMA has been calculated for volatilisation from a model river. In soil, *n*-BMA is characterised by moderate adsorption, while *i*-BMA was found to be strongly adsorbed.

n-BMA/*i*-BMA is of moderate toxicity (EC₅₀: 10-100 mg/l) to bacteria, fish and *Daphnia*. *i*-BMA had a high toxicity (> 0.1 mg/l) towards green algae when tested in a closed system based on a 96-h NOEC of 0.047 mg/l. However, this effect was reversible and represented an algal static rather than an algalicidal action of *i*-BMA. When tested in a standard open test system the toxicity of *n*-BMA to green algae could not be measured conclusively because of the rapid loss of the material during the exposure time. The test results of the algae studies indicate that the hazard identified by the growth inhibition observed with *i*-BMA in a closed system should be viewed in the light of the reversibility of the effect and the probable volatilisation under open exposure conditions which represent more closely the normal environmental situation. This accounts for the lower toxicity of *n*-BMA observed in an open test system.

From the physico-chemical data it is anticipated that *n*-BMA/*i*-BMA is rapidly absorbed after oral or inhalation exposure. *In vitro* studies using isolated rat liver microsomes or porcine liver esterase showed rapid hydrolysis of *n*-BMA yielding methacrylic acid and *n*-butanol. No *in vivo* metabolism data are available on *n*-BMA/*i*-BMA, but from the *in vitro* data rapid hydrolysis to methacrylic acid and the corresponding alcohol can be anticipated. *n*-BMA did not bind to glutathione (GSH) *in vitro*. It is expected that after hydrolysis the respective cleavage products methacrylic acid and *n*-butanol or

isobutanol are further metabolised by normal physiological pathways ultimately to CO₂. The interpretation of the toxicological data is based on these assumptions.

In mammals *n*-BMA/*i*-BMA is of low acute toxicity by the oral, dermal or inhalation route of exposure. They have local irritating properties to rabbit skin and eyes. Respiratory tract irritation was observed after inhalation exposure of rats to *n*-BMA. Although no data on respiratory irritation are available for *i*-BMA it is expected to have similar effects as *n*-BMA. Whilst *n*-BMA is a weak skin sensitiser in guinea pigs, there is no such evidence for *i*-BMA. From the available human clinical data it can be concluded that the sensitisation potential to humans of *n*-BMA is low.

A repeat dose oral study in mice is available which, although of limited reliability, indicates that *n*-BMA is of low oral toxicity. A reliable 28-day exposure inhalation study in rats is available for *n*-BMA. The lead effect in this study was the formation of nasal lesions indicative of a local irritant effect in the olfactory region of the nose with no indications of systemic toxicity.

Neither *n*-BMA nor *i*-BMA was mutagenic in a number of gene mutation assays with *Salmonella typhimurium*. *i*-BMA was not clastogenic in a mouse micronucleus assay. Despite the rather limited database, taking into account the close structural similarity of the two isomers and data on other methacrylic acid esters, there is no immediate concern for genotoxicity.

For the endpoints carcinogenicity, chronic toxicity and toxicity to reproduction, no reliable data are available for either ester. However, information concerning potential hazards of *n*-BMA/*i*-BMA may in part be inferred from studies with methyl methacrylate which like *n*-BMA/*i*-BMA is metabolised to methacrylic acid in animals and in humans.

Given the lack of carcinogenicity observed with methyl methacrylate and the lack of genotoxic potential of *n*-BMA/*i*-BMA, there is no immediate concern with regard to a possible carcinogenic potential of *n*-BMA/*i*-BMA. The Task Force is not aware of any reliable data on the carcinogenicity of *n*-butanol and isobutanol.

With regard to chronic toxicity the lead effect for methyl methacrylate long term inhalation exposure was local nasal irritation. The lead effect in a 28-day *n*-BMA study is consistent with this pattern of toxicity and therefore suggests that this study is an appropriate and relevant indicator of chronic toxicity.

Due to the paucity of data, no firm conclusions can be made on the potential toxicity to reproduction. However, the data available for methyl methacrylate and *n*-butanol and isobutanol suggest that there

is no need for immediate concern for possible developmental effects arising from inhalation exposure to non-maternally toxic concentrations of *n*-BMA/*i*-BMA.

Limited data available from repeated dose studies with *n*-BMA, methyl methacrylate, methacrylic acid and a fertility study with *n*-butanol did not reveal any indications for possible toxic effects on the reproductive organs.

The sensitisation potential of *n*-BMA to humans is low.

Despite the use of *n*-BMA/*i*-BMA for many years, no adverse systemic health effects have been observed. The lead effect of *n*-BMA/*i*-BMA identified in acute and subchronic animal studies is the local irritation at the site of contact following exposure by the inhalation route, the major route of occupational exposure. From the available studies it can be concluded that upper respiratory tract irritation is the most common effect of inhalation exposure to *n*-BMA/*i*-BMA.

2. IDENTITY, PHYSICAL AND CHEMICAL PROPERTIES,

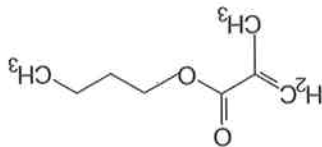
ANALYTICAL METHODS

2.1 IDENTITY

2.1.1 *n*-Butyl Methacrylate

Name:	<i>n</i> -Butyl methacrylate (<i>n</i> -BMA)
IUPAC name:	Butyl 2-methyl-2-propenoate
Synonyms:	Butyl 2-methacrylate 2-Methyl-2-propenoate, butyl- Methacrylic acid, butyl ester
Danish:	Butylmethacrylat
Dutch:	<i>n</i> -Butylmethacrylaat
Finnish:	2-Methylbutylacrylaatti
French:	Méthacrylate de butyle
German:	<i>n</i> -Butylmethacrylat
Greek:	Μεθ ακρυλικός <i>n</i> -βουτυλαεστεράς
Italian:	<i>n</i> -Butilmetacrilato
Norwegian:	Butylmetakrylat
Portuguese:	Metacrilato de <i>n</i> -butilo
Spanish:	Metacrilato de butilo
Swedish:	Butylmetakrylat
CAS name:	2-Propenoic acid, 2-methyl-, butyl ester
CAS registry No:	97-88-1
EEC No:	607-033-00-5
EEC classification:	Irritant
EEC labelling:	Symbol irritant (Xi), R10-36/37/38-43, nota D
EINECS No:	202-615-1
Formula:	C ₈ H ₁₄ O ₂
Molecular mass:	142.20

Structural formula:



2.1.2 Isobutyl Methacrylate

Name: Isobutyl methacrylate (*i*-BMA)

IUPAC name: Isobutyl 2-methylpropenoate

Synonyms:

Isobutyl 2-methylacrylate
Isobutyl 2-methyl-2-propenoate
Methacrylate, 2-methylpropyl ester
Methacrylic acid, isobutyl ester
2-Methyl-2-propenoic acid, 2-methylpropyl ester
2-Methylpropyl methacrylate
Propenoic acid, 2-methyl, isobutyl ester

Danish:

Isobutylmethacrylat

Dutch:

Isobutylmethacrylaat

Finnish:

Isobutyyli metakrylaatti

French:

Méthacrylate de d'isobutyle

German:

Isobutylmethacrylat

Greek:

Μεθακρυλικός ισοβουτυλαεστέρας

Italian:

Isobutilmetacrilato

Norwegian:

Isobutylmetakrylat

Portuguese:

Metacrilato de isobutilo

Spanish:

Metacrilato de isobutilo

Swedish:

Isobutylmetakrylat

CAS name:

2-Propenoic acid, 2-methyl-, 2-methylpropyl ester

CAS registry No:

97-86-9

EEC No:

607-113-00-X

EEC classification:

Irritant

EEC labelling:

Concentration \geq 20 %: symbol irritant (Xi), R 10-36/37/38-43;

S 24-37, nota D

1 % \leq concentration < 20 %: symbol irritant (Xi), R43

EINECS No:

202-613-0

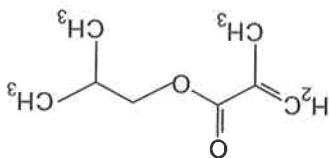
Formula:

$C_8H_{14}O_2$

Molecular mass:

142.20

Structural formula:



2.2 PHYSICAL AND CHEMICAL PROPERTIES

At room temperature, *n*-BMA/*i*-BMA is a clear, colourless, flammable liquid with a faint characteristic ester odour. Both compounds have a low solubility in water and are soluble in most organic solvents. Data on the physical and chemical properties of *n*-BMA/*i*-BMA are given in Table 1 and 2.

n-BMA

A typical commercial sample of *n*-BMA has a specified purity of $\geq 99.0\%$ (w/w) and contains water (0.05% w/w) and other impurities. The identity of these impurities will vary depending on the production process (Section 3.1) and may include traces of methacrylic acid and methyl methacrylate.

i-BMA

A typical commercial sample of *i*-BMA has a specified purity of $\geq 98.5\%$ (w/w) and contains water (≤ 0.01 - 0.02% , maximum 0.1% w/w) and other impurities. The identity of these impurities will vary depending on the production process (Section 3.1) and may include traces of methacrylic acid and methyl methacrylate.

n-BMA/*i*-BMA

n-BMA/*i*-BMA polymerises readily under the influence of heat, light or by catalysis (e.g. metals and radical forming substances such as peroxides), this being a strongly exothermic reaction. To prevent polymer formation, the monomer is stabilised by the addition of inhibitors such as 2-(1,1-dimethylethyl)-4,6-dimethylphenol (10-100 ppm, maximum $< 0.1\%$ w/w), hydroquinone (HQ) (10-100 ppm, maximum $> 0.1\%$ w/w) and the monomethylether of hydroquinone (MeHQ, synonym *p*-methoxyphenol) (10-100 ppm, maximum $> 0.1\%$ w/w).

Table 1: Physical and Chemical Properties of *n*-BMA

Parameter, units	Value	Reference
Melting temperature, °C, approximately	-25	Company data sheets ^a
Boiling temperature, °C at 1,013 hPa	160-163	Company data sheets ^a ; Weast <i>et al</i> , 1989; Bauer, 1993
Relative density D ₄ ²⁰	0.896-0.8975	Nemec and Krich, 1981
Viscosity, mPa·s at 20 °C	1.1-1.2	Company data sheets ^a
at 21 °C	3.116	HSDB, 1994
Refractive index, n _D at 20 °C	1.422	Kirk-Othmer, 1981
Vapour pressure, hPa at 20 °C	2.40	Company data sheets ^a
	6.1	HSDB, 1994
	4.8	HSDB, 1994
Vapour density at 20 °C (air=1)	0.015-0.06	Company data sheets ^a
Threshold odour concentration, ppm	0.025	Shepel'skaya, 1978
Surface tension, mN/m at 20 °C	35	HSDB, 1994
Solubility in water, g/kg at 20 °C	> 0.45	Company data sheets ^a
	0.882 ^b	Lissi <i>et al</i> , 1983
Solubility of water in <i>n</i> -BMA, g/kg at 20 °C	0.04	Company data sheets ^a
Miscible with most organic solvents	Yes	Company data sheets ^a ; HSDB, 1994
Fat solubility, mg/100 g at 37 °C	No data	
Partition coefficient, log P _{ow} (octanol/water), measured at 20 °C	2.6 ^b	Fujisawa and Masuhara, 1981; Dillingham <i>et al</i> , 1983
	2.88 ^b	Tanii and Hashimoto, 1982
	3.01 ^b	Morris <i>et al</i> , 1992a
	2.26 ^c	Fujisawa and Masuhara, 1981
Partition coefficient, K _{oc} (organic carbon/water), calculated at 20 °C	74.8-421	According to CEC, 1994a
at 25 °C	878 ^e	Swann <i>et al</i> , 1983
	63.6	According to SRC, 1994
	11 ^f	Hine and Mokerjee, 1975
	46	Röhm, 1995a
	49	Degussa, 1968
Explosion limits, % at 65-96 °C and 1,000 hPa	2-8	Company datasheets ^a ; HSDB, 1994
Auto-flammability, ignition temperature, °C	315	Degussa, 1990
	400-496	Degussa, 1968

a Rohm and Haas, 1993; ICI Acrylics, 1994; Degussa, 1995a; Röhm, 1996a

b Shake flask method

c High performance liquid chromatography (HPLC) method

d Based on log P_{ow} = 2.26-3.01

e Based on log P_{ow} of 2.88 and regression equation of Lyman *et al* (1982)

f Calculated; reported as 1.09x10⁻⁴ atm·m³/mol

Table 2: Physical and Chemical Properties of *t*-BMA

Parameter, units	Value	Reference
Melting temperature, °C	-37 - -34	Company data sheets ^a
Boiling temperature, °C at 1,013 hPa	155	Deichman, 1981; West et al, 1989; Richter et al, 1961; Company data sheets ^a
Relative density D ₂₀ ⁴	0.882-0.888	Degussa, 1989; Nemeč and Kirch, 1981; Rehberg and Fisher, 1948; Richter et al, 1961; West et al, 1989; Company data sheets ^a
Viscosity, mPa·s at 20 °C	0.9	Company data sheets ^a
Refractive index, n _D at 20 °C	1.4197-1.420	Nemeč and Kirch, 1981; Degussa, 1989
Vapour pressure, hPa at 20 °C (air=1)	2.4-4	Deichman, 1981
Vapour density at 20 °C	4.9	Deichman, 1981
Threshold odour concentration, ppm	0.016-0.069	ICI Acrylics, 1994
Surface tension, mN/m at 24 °C	23.5 ^b	DIPPR, 1995
Solubility in water, g/kg at 20 °C	0.133	Mao, 1995
Solubility of water in <i>t</i> -BMA, g/kg at 20 °C	0.005	Röhm, 1995b
Miscible with most organic solvents	Yes	West et al, 1989; ICI Acrylics, 1994
Fat solubility, mg/100 g at 37 °C	No data	
Partition coefficient, log P _{ow} (octanol/water), measured at 20 °C	2.66 ^c	Tanii and Hashimoto, 1982
Partition coefficient (soil), K _{oc} (organic carbon/water) at 20 °C	2.01 ^d	Fujisawa and Masuhara, 1981
Partition coefficient (soil), K _{oc} (organic carbon/water) at 20 °C	1480-3920	Christensen, 1995a
Flash point, °C, closed cup (DIN 51755)	42.05-171.3	Calculated according to CEC, 1994a
Explosion limits, % at 25 °C and 1,013 hPa	1-7.4	DIPPR, 1995
Auto-flammability, ignition temperature, °C	ca. 2-8	Degussa, 1995a,b
	367-400	Company data sheets ^a ; Degussa, 1994

a Elf Atochem, 1993; ICI Acrylics, 1994; Degussa, 1995b,c; Röhm, 1996b

b Calculated according to Sugden, 1924

c Shake flask method

d High performance liquid chromatography (HPLC) method

2.3 CONVERSION FACTORS

Conversion factors for concentrations of *n*-BMA and/or *t*-BMA in air at 20 °C and 1,013 hPa are:

■ 1 ppm = 5.91 mg/m³

■ 1 mg/m³ = 0.169 ppm

2.4 ANALYTICAL METHODS

n-BMA/*i*-BMA may be analysed and detected by common chromatographic techniques as reviewed by Nemeč and Kirch (1981) e.g. gas chromatography (GC) or high performance liquid chromatography (HPLC). These techniques are used for assaying the purity of methacrylate monomers, monomer content in mixtures with other monomers, in solutions and (residual levels) in polymers.

2.4.1 Purity of *n*-BMA/*i*-BMA

n-BMA/*i*-BMA can be assayed for purity by capillary gas chromatography (GC) using a flame ionisation detector (FID) (Röh, 1993a). Impurities present in concentrations of 10 ppm or higher may be identified and quantified by coupled mass spectrometry (GC/MS) and calibration of the peak area.

2.4.2 *n*-BMA/*i*-BMA in Products

Residual Monomer

Residual *n*-BMA/*i*-BMA in polymeric products can be determined by GC headspace analysis. The material under investigation is dissolved in or extracted with a solvent of low volatility like dimethylformamide. Subsequently the sample is equilibrated at elevated temperature and analysed by GC/FID (Röh, 1993b). With a *n*-BMA/*i*-BMA copolymer the quantitation limit was determined to be 2 ppm. This method may also be used for the determination of residual monomer concentrations in dispersions/emulsions.

Residual *n*-BMA/*i*-BMA in aqueous polymer emulsions was determined by GC (Miller and Harper, 1983). The samples were analysed by direct injection or following extractive distillation with cyclohexane. The extraction method showed better reproducibility and precision.

Mixtures and Polymers

Mass spectrometry (MS) has been used to identify *n*-BMA, and other acrylic monomers in resin-based dental materials (Gjoes *et al*, 1983). The materials were either injected directly or dissolved in dichloromethane to separate solid filler materials. Mass spectra were determined for most components of dental resins.