

Effects of Ingredients on Cigarette Smoke Composition and Biological Activity: A Literature Overview*

by

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SUMMARY

This paper presents a literature review of published scientific studies of the effects of tobacco product ingredients and various experimental additives on cigarette smoke composition and its biological activity. The format of this work is that of an uncommented reference paper rather than a critical scientific review. Therefore, the mention of an ingredient in this survey does not imply that it is used by the tobacco industry or that it is covered by any existing na-

tional regulations. A broad range of scientific papers and patents on tobacco ingredients is included as well as studies on experimental ingredients.

This review may provide public health officials as well as scientists in government agencies and in the tobacco industry with a helpful overview of published information on tobacco product ingredients, their transfer into mainstream cigarette smoke, pyrolysis products, and influence on the biological activity of mainstream cigarette smoke. [Beitr. Tabakforsch. Int. 20 (2002) 107–247]

ZUSAMMENFASSUNG

Bei der vorliegenden Publikation handelt es sich um eine Literaturübersicht über publizierte wissenschaftliche Studien, die die Auswirkungen von gebräuchlichen Zusatzstoffen und auch von verschiedenen experimentellen Additiven zu Cigaretten auf die chemische Zusammensetzung oder auf die biologische Aktivität des Rauches untersucht haben. Da das Format dieser Arbeit eher das einer unkommentierten Zusammenstellung publizierter Daten als das eines kritischen Übersichtsartikels ist, soll an dieser Stelle darauf hingewiesen werden, dass die Erwähnung eines Zusatzstoffes nicht bedeutet, dass er von der Tabakindustrie verwendet oder dass er durch irgendeine nationale Regulierung erfasst wird. Neben einer Vielzahl von wissenschaftlichen Publikationen und Patenten über verwendete Zusatzstoffe wurden auch Daten aus zahlreichen Studien über experimentelle Zusatzstoffe aufgenommen.

Das Ziel dieses Reviews ist, sowohl den Gesundheitsbehörden als auch Wissenschaftlern in Regierungseinrichtungen und in der Tabakindustrie einen schnellen Überblick über publizierte Informationen zu Additiven, ihren Übergang in den Hauptstromrauch, ihre Pyrolyse und auch ihren Einfluss auf die biologische Aktivität des Hauptstromrauches zu geben. [Beitr. Tabakforsch. Int. 20 (2002) 107–247]

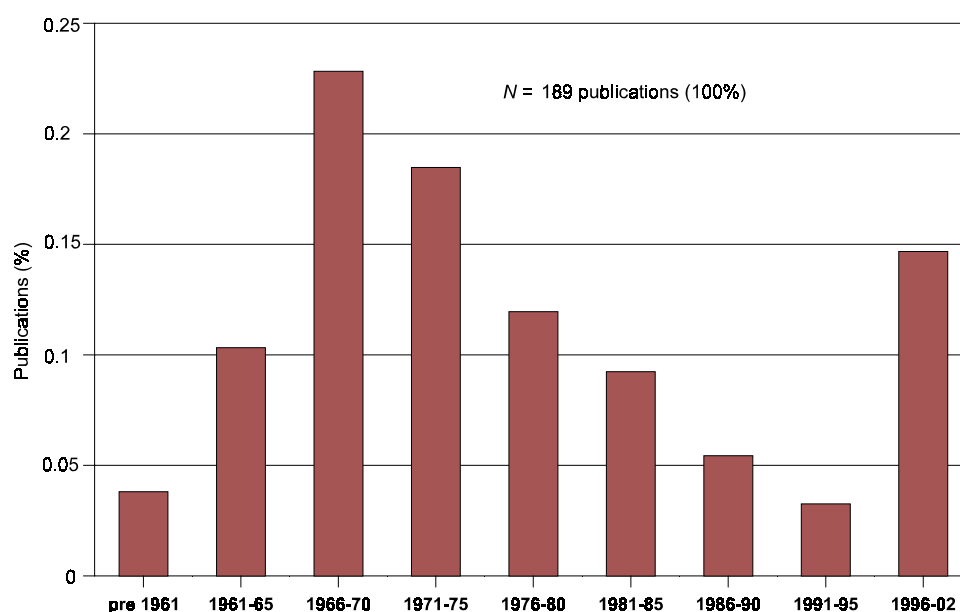


Figure 1. Temporal distribution of publications dealing with additives

RESUME

Cette étude est une revue de la littérature scientifique sur les effets des composants des produits du tabac et de divers additifs expérimentaux sur la composition de la fumée du tabac et de son activité biologique. Cette étude est présentée sous forme d'une liste de références non commentées plutôt que d'une revue scientifique critique. Pour cette raison, la mention dans cette revue d'un composant ne signifie pas qu'il est apporté au tabac ou qu'il fait l'objet d'une réglementation nationale. Cette revue examine une vaste gamme de publications scientifiques et brevets sur les composants des produits du tabac et des études sur les additifs expérimentaux.

Cette revue peut donc fournir aux autorités de la santé publique, ainsi qu'aux chercheurs des institutions gouvernementales et de l'industrie du tabac, un bref aperçu des informations publiées sur les composants des produits du tabac, leur transfert dans la fumée du courant principal, leurs produits de pyrolyse et leur influence sur l'activité biologique de la fumée du courant principal. [Beitr. Tabakforsch. Int. 20 (2002) 107–247]

INTRODUCTION

The use of certain additives, in particular the use of those claimed to enhance nicotine delivery to smokers, has been subject to extensive debate (Action on Smoking and Health [ASH] 1999, Müller and Röper 2000). Although most substances employed as additives in cigarette manufacture are “generally recognised as safe” (GRAS) for use in foods and/or listed on the Flavour and Extract Manufacturers Association's (FEMA) GRAS list, they may yield unknown pyrolysis products on combustion if used in to-

bacco products. The fact that an ingredient is GRAS does not mean that it is safe, or has been approved for use, in tobacco products.

Nowadays, different forms of regulations and disclosures exist in several countries of the European Union (e.g., France, the United Kingdom and Germany) as well as in the United States (list of 599 ingredients [TR Staff Report, 1994]), which control the use of ingredients for the manufacture of tobacco products.

In a directive of the European Parliament and of the Council concerning the manufacture, presentation and sale of tobacco products, an ingredient is defined as “any substance except for tobacco leaf and other natural or unprocessed tobacco plant parts used in the manufacture and preparation of a tobacco product and still present in the finished product, even if in altered form, including paper, filter, inks and adhesives” (EU-Directive 2001/37/EC, Article 2 (5)).

This literature review was compiled to provide an overview of the published data concerning the effects of ingredients on smoke composition and its biological activity. More than 10,000 literature search hits were evaluated for their relevance for inclusion in this review according to the criteria defined in the section “Materials and Methods”. The 189 reports thus selected form the basis for the evaluation of the ingredients in Tables 2 to 7 (see Appendix). This literature can be divided into two categories: The major part of the published literature is concerned with the chemical identification and detection of the pyrolysis products of tobacco ingredients (Tables 3 to 5), while Tables 6 and 7 deal with studies evaluating toxicological aspects of the burned ingredients. In general, it can be seen that many papers on the topic of ingredients were published between 1965 and 1975, after which the frequency of publications gradually dropped and only increased again from 1995 onwards (see Figure 1).

Table 1. Classification of ingredients and their functions

Ingredient	Classification	Function
Flavourings, casings	1	Improvement of organoleptic properties
Humectants	2	Improvement of moisture retention and elasticity of the leaf
Burn additives	3	Improvement of ash appearance, whiteness and burn uniformity
Plasticisers	4	For printing of colours on cigarette papers, cigarette filter wrappers, tips and filter tips
Preservatives, stabilisers	5	Improvement of product shelf life
Adhesives, thickening agents, fillers	6	Needed for the seam, the plug wraps, the tips and filter tippings, and for reconstituted tobacco sheet
Dyes	7	Needed for imprints on cigarette paper or paper for tips and filter tips
Processing aids, solvents	8	Auxiliary materials for the manufacturing process
Experimental additives	9	Not known to be used as ingredients on cigarette tobacco

FUNCTION OF INGREDIENTS

Although the tobacco leaf is primarily responsible for the taste and flavour of tobacco smoke, certain ingredients when combined in a unique, proprietary manner, provide each brand with its own unique flavour, taste and aroma (Gutcho, 1972). About three decades ago, LEFFINGWELL *et al.* (1972) reviewed the use of flavouring components in smoking products.

The classification used in terms of the function of the ingredients is shown in Table 1. All ingredients dealt with in this review were assigned to one or more of these nine classes (Table 2). The approach taken is meant to be informative and pragmatic rather than authoritative.

MATERIALS AND METHODS

Literature search

A wide search algorithm was used which included the terms “flavo(u)”, “additive”, “aroma”, “cigarette”, “smoking” or “tobacco” as well as the names of individual substances covered for example by the German Tobacco Ordinance (Tabakverordnung No. 360, German TVO) or contained in the list of 599 ingredients for use in the manufacture of cigarettes sold in the USA submitted to the US Department of Health and Human Services (TR Staff Report, 1994). This search algorithm was used to examine:

- In-house databases
- Medical databases such as Medline, Embase, Somed and Biotechnobase

- Toxicological databases such as Toxline and Toxcas
- Chemical database clusters such as Analytical Chemistry and Chemical Engineering (which also contains Chemical Abstracts and patents).

Using the above search algorithm, over 10,000 hits for research papers, reports and patents were obtained. Information provided in patents and research papers has to be treated with caution since this does not necessarily imply use by the tobacco industry.

Inclusion criteria

Only those publications were considered in which the influence of the ingredients applied to tobacco on the properties and composition of the mainstream smoke was investigated. Also included were studies which investigated the pyrolysis products of ingredients or mixtures of ingredients. Papers that analysed ingredients in unpyrolysed form were not included, such as those used in quality control to determine the stability of an ingredient during cigarette storage. Studies concerned with new filter technologies or those dealing with filter materials such as cellulose acetate or non-volatile compounds and salts added in the filter were not included because these substances are not expected to appear in mainstream smoke. Publications reporting the effect of ingredients only on the burn characteristics of tobacco and changes only in the organoleptic properties of tobacco smoke were also excluded.

For studies reporting toxicological effects of ingredients, an additional selection criterion was used. Publications which analysed only the toxicological effects of ingredients (in unchanged or pyrolysed form) independently of their application to tobacco were not considered.

RESULTS

All ingredients covered in this review are listed in alphabetical order in Table 2, which can be used as an index. The entries in columns 3 to 6 of Table 2 indicate whether the ingredient was investigated as a single compound (S) or in a mixture (M 1 – M 65). Experimental additives are marked with grey shading.

For each individual ingredient, the following information is provided: Function, as classified in Table 1; data in mainstream smoke (Tables 3 and 4); pyrolysis data (Table 5); data of biological activity in mainstream smoke (Tables 6 and 7).

Mainstream smoke

Table 3 contains information on the influence of ingredients on the chemical composition of cigarette mainstream smoke.

More than 150 different ingredients are cited and alphabetically listed. The reported ingredients have been applied either to the tobacco filler, the finished product, to the cigarette paper, or used as components in the manufacture of reconstituted tobacco sheets. The column “Amount” contains information on the amount of ingredients in the relevant end product. The form in which the ingredients were applied differed widely, depending on the experimen-

tal design and the materials used. It ranged from spraying ingredient solutions onto the tobacco filler, injection of ingredients into the tobacco rod of cigarettes or impregnating cigarette paper with a solution of ingredients. Whenever possible, transfer data into the smoke are listed, pyrolysis products and their concentrations are registered, or their influence on other mainstream smoke components is stated. Whenever a percentage is given for a smoke component it generally signifies an increase (↗) or decrease (↘) compared to control cigarettes without the ingredient(s). Based on the structure of Table 3, a further list of mixtures of ingredients is presented (Table 4). Many ingredients are incorporated into cigarettes in the form of mixtures, in many cases as components of reconstituted tobacco.

The evaluated literature revealed 61 different combinations of ingredients as listed in Table 4 and labelled as M 1 – M 58, M 62, M 63 and M 64. In this Table, the published data for the combinations of ingredients are listed alphabetically by the author's name. Most of the mixtures (M1 – M 59, M 65) are listed with their relevant ingredients in Tables 4, 6 and 7. The composition of mixtures M 60 – M 64 is not given in detail. The list of ingredients for these mixtures can be found in the original literature or can be extracted from Table 2.

The column "Amount" in Table 4, in contrast to Table 3, does not always give information on the amount of ingredients in the relevant end product. In some cases data in this column refer to the portion of single ingredients within the mixture.

Pyrolysis

Table 5 summarises the results of pyrolysis experiments performed with tobacco and cigarette ingredients. Furthermore, this table contains information on the experimental pyrolysis conditions used, the percentage of unchanged material in the pyrolysate as well as qualitative and quantitative data on the pyrolysis products formed. The analytical pyrolysis experiments do not predict with certainty which materials will be produced when the ingredient is added to a cigarette and burned, but provide some insight of what may be produced. Table 5 has 161 entries, corresponding to 104 different "single"¹ ingredients.

Since no standardised conditions exist for the investigation of ingredient pyrolysis, most experimental conditions were chosen to simulate the temperature conditions found in a burning cigarette, both during and between puffs. However, the pyrolysis conditions actually used varied widely. The temperature ranged from 50 to 900 °C, with approximately 700 °C most frequently used. In most investigations, the ingredient (or mixture of ingredients) was pyrolysed without adding any carrier substances. In some studies, the ingredient was mixed with Celite as a carrier (Robb *et al.*, 1964). The duration of pyrolysis was most frequently between 1 and 10 min. Some pyrolysis studies were performed until the test material had disappeared.

Pyrolytic experiments were performed in streams of air, nitrogen or helium. The gas flows, when given, ranged from 15 mL/min to 1.5 L/min.

It should be mentioned that the investigations of KRÖLLER, a scientist at the former German Federal Health Office (Bundesgesundheitsamt, BGA, which was responsible for the regulation of tobacco ingredients in Germany) contribute the vast majority of the pyrolysis data on tobacco ingredients in Table 5 (KRÖLLER investigated 58 different ingredients constituting about a third of all entries and more than half of all ingredients listed in Table 5).

Data on the percentage of unchanged ingredients in the pyrolysate are scarce. In the first place, data are available for ingredients which are designed to release the desired additive when heated (e.g., Robb *et al.*, 1964; Southwick, 1992). In addition, quantitative data on unchanged ingredients in the pyrolysate (primarily for humectants) are available from the investigations of KRÖLLER (Kröller, 1964b, 1970).

Most of the results of pyrolysis experiments with tobacco ingredients deal with thermal decomposition products, primarily those which are of relevance for the toxicological and flavour properties of the ingredient. KRÖLLER was primarily interested in the assumed toxicological properties of tobacco ingredients when he analysed the pyrolysate for polycyclic aromatic hydrocarbons (PAHs), quinones, phenols and aldehydes. For some constituents, e.g. benzo[*a*]pyrene (B[*a*]P), quantitative data (expressed as µg/100 g ingredient pyrolysed) are available. In a series of pyrolysis experiments, SCHLOTZHAUER investigated primarily mono- and polysaccharides as well as amino acids and proteins for their potential to form phenols and aldehydes or N-heterocyclic compounds and nitriles, respectively (Schmeltz *et al.*, 1972; Schlotzhauer *et al.*, 1982, 1986). The remaining studies shown in Table 5 also focussed their attention on the pyrolytic formation of toxic substances from ingredients.

Biological activity

The literature search identified a total of 37 publications in which the change in biological activity of cigarette smoke due to the application of ingredients was studied (Tables 6 and 7). Table 6 contains publications reporting studies on ingredients which are, or could be, used in the manufacturing process, while Table 7 presents publications on experimental ingredients.

The fact that cigarette smoke itself is biologically active means that a high level of sensitivity is required in the test systems to detect changes in toxicological endpoints. The selected publications used the assays listed in Table 8 to study the effect of ingredients on the biological activity of cigarette smoke or cigarette smoke condensate.

The majority of the ingredients listed in Tables 6 and 7 were systematically investigated for their biological activity in just a few studies (Gaworski *et al.*, 1998, 1999b; Römer *et al.*, 2002; Vanscheeuwijck *et al.*, 2002). In these studies, ingredients were added to cigarettes in different mixtures at realistic concentrations and, where technically possible, also at higher levels. In none of the studies listed in Table 6 was the biological activity of cigarette smoke found to be increased due to application of the ingredient mixtures,

¹"Single" additive does not necessarily mean an individual substance. In many cases extracts from natural products forming complex mixtures were used as an additive.

Table 8. Assays used to determine biological activity of cigarette smoke

Assay	Toxicological endpoint	Tested agent	References
Mouse skin-painting assay	Tumorigenicity	CSC ^a	BOCK <i>et al.</i> , 1974; COLLINS <i>et al.</i> , 1981; DONTENWILL <i>et al.</i> , 1972, 1976; GARGUS <i>et al.</i> , 1975; GAWORSKI <i>et al.</i> , 1999a; HALTER and ITO, 1972; HOFFMANN and WYNDER, 1967, 1968, 1972; NCI Report No. 1, 1976; No. 3, 1977; No. 4, 1980; RÖMER and HACKENBERG, 1990; TSO, 1975; WYNDER and HOFFMANN, 1961, 1969
Ames assay	Mutagenicity	CSC ^a	KIER <i>et al.</i> , 1974; MCCOY and ROSENKRANZ, 1982; RÖMER <i>et al.</i> , 2002; SATO <i>et al.</i> , 1979; BOMBICK <i>et al.</i> , 2001
Inhalation studies using rodents	Tumorigenicity, other toxicological endpoints such as decrease in weight gain, changes in tissue and cell properties	Tobacco smoke	DONTENWILL, 1974; GAWORSKI <i>et al.</i> , 1997, 1998, 1999b; JONES <i>et al.</i> , 1972, 1973; VANSCHEEUWIJCK <i>et al.</i> , 2002; MISRA <i>et al.</i> , 2001
<i>In vivo</i> and <i>in vitro</i> ciliotoxicity	Ciliostasis, inhibition of particle clearance	Tobacco smoke	DALHAMN, 1969; DALHAMN and Rylander, 1971; NCI Report No. 1, 1976; No. 3, 1977; No. 4, 1980; RAKIETEN, 1952; RYLANDER, 1971, 1973
Cytotoxicity in cell cultures	Growth inhibition, cell viability	CSC ^a	RÖMER <i>et al.</i> , 2002; NCI Report No. 1, 1976; No. 3, 1977; No. 4, 1980; BOMBICK <i>et al.</i> , 2001
<i>In vitro</i> macrophage inhibition assay	Inhibition of macrophage activity	Tobacco smoke	NCI Report No. 1, 1976
Chemical analysis	Determination of risk indices	Tobacco smoke	RUSTEMEIER <i>et al.</i> , 2002
Sister-chromatid exchange in cell cultures	Cytogenetic endpoint	CSC ^a	BOMBICK <i>et al.</i> , 2001

^aCSC = cigarette smoke condensate.

whereas the addition of ingredients under experimental conditions in some cases lead to an increase in biological activity (NCI Report No.1, 1976; No. 3, 1977; Wynder and Hoffmann, 1961; Hoffmann and Wynder, 1968; Kier *et al.*, 1974; McCoy and Rosenkranz, 1982) (Table 7).

A number of ingredients such as cocoa, glycerol, menthol or sugar are used at considerably higher inclusion levels than most flavour additives and have been subject to extensive toxicological testing (NCI Report No. 3, 1977; Römer and Hackenberg, 1990; Gaworski *et al.*, 1997, 1999b; Sato *et al.*, 1979; Carmines, 2002; Römer *et al.*, 2002; Vanscheeuwijck *et al.*, 2002). Except for one study by the National Cancer Institute (NCI Report No. 3, 1977) in which the addition of 1% cocoa to test cigarettes led to an increase in tumorigenicity of mainstream smoke condensate in the mouse skin painting assay, other studies have shown no increase in biological activity of mainstream cigarette smoke condensate from test cigarettes. The findings of the NCI study could not be confirmed in another study in which addition of 1% or 3% cocoa to cigarette tobacco filler did not result in an increase in mainstream smoke condensate tumorigenicity in mouse skin painting assays (Römer and Hackenberg, 1990). The authors explained the contradictory results by the fact that a control group used in the NCI study exhibited an unusually low tumour incidence in comparison with other controls.

Although the results of the NCI study with respect to an increase in tumorigenicity due to the addition of cocoa to cigarettes were not statistically significant (NCI Report No. 3, 1977), the British Government reacted to this publication by prohibiting the addition of cocoa to tobacco products (Glantz, 1996). However, in view of new toxicological data

submitted to the UK Independent Scientific Committee on Smoking and Health the prohibition was removed in 1983 and the addition of up to 5% cocoa allowed in tobacco products (Glantz, 1996).

CONCLUDING REMARKS

This compilation clearly reveals that experimental investigations on tobacco product ingredients are rather heterogeneous. The majority of ingredients have been evaluated for biological activity and most of these studies clearly indicate that ingredients do not increase the biological activity of cigarettes. It is obvious that a lot of gaps exist in our knowledge on the pyrolysis and potential transfer of tobacco product ingredients to mainstream cigarette smoke. Perhaps the most compelling conclusion from this literature survey is the need for generally accepted (standard) methods for the investigation of tobacco product ingredients and their influence on the properties of mainstream cigarette smoke.

GLOSSARY (Tables 2 to 7)

A	= abstract
act.	= activity
aliph. hydrocarb.	= aliphatic hydrocarbons
B[a]A	= benz[a]anthracene
B[a]P	= benzo[a]pyrene
B[e]P	= benzo[e]pyrene
CA	= cellulose acetate

CF	= Cambridge filter
CH	= charcoal + cellulose acetate
cig.	= cigarette
CMC	= carboxymethyl-cellulose
colorim.	= colorimetric
cond.	= condition
CSC	= cigarette smoke condensate
DAP	= diammonium phosphate
DNP	= 2,4-dinitrophenol
DPM	= dry particulate matter
FF-M	= full flavour menthol
FFLT-M	= full flavour low "tar" menthol
max.	= maximum
min.	= minimum
MSS	= mainstream smoke
n.d.	= not determined
n.r.	= not reported
NAB	= <i>N</i> -nitrosoanabasine
NAT	= <i>N</i> -nitrosoanatabine
NCI	= National Cancer Institute
NDMA	= <i>N</i> -nitroso-dimethylamine
NFDPM	= nicotine free dry particulate matter
NNK	= 4-(<i>N</i> -methyl- <i>N</i> -nitrosamino)-1-(3-pyridyl)-1-butanone
NNN	= <i>N</i> -nitrososornicotine
NO _x	= nitrogen oxides
NPYR	= <i>N</i> -nitrosopyrrolidine
OLL	= oleic, linoleic, linolenic acids
P	= patent
PAH	= polycyclic aromatic hydrocarbons
PHB	= polybetahydroxy butyric acid
PMO	= phenyl-methyl-oxadiazole
RT	= reconstituted tobacco
SB	= standard blend
SEB	= standard experimental blend
synth.	= synthetic
tot.	= total
tot. w-acids	= total weak acids
TPM	= total particulate matter
ULT-M	= ultra low "tar" menthol
v/v	= volume/volume
w/w	= weight/weight

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Table 2: Overview of ingredients mentioned in the literature

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Acetanisole	1	M 62, 63	S	M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Acetic acid	3			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Kröller, 1966b Carmines, 2002 ^c
Acetoin	1	M 62, 63		M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Acetophenone	1	S		M 61 M 60		Bavley and Robb, 1969 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Acetylpyrazine	1	M 62, 63		M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2-Acetylthiazole	1	M 63		M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Aconitic acid	1	M 63		M 63		Carmines, 2002 ^c
Adipic acid	9	M 28				Komatsu, 1997
Agar-agar	6		S S			Kröller, 1965b Sjöberg and Pyysalo, 1985
Alanine	1	S		M 61		Kaburaki <i>et al.</i> , 1969 Gaworski <i>et al.</i> , 1998
Alfalfa extract	1	M 62		M 62		Carmines, 2002 ^c
Alginate acid	6		S S			Kröller, 1965b Sjöberg and Pyysalo, 1985
Allspice oil	1	M 62		M 62		Carmines, 2002 ^c
Aluminium oxide	3				S S	Hoffmann and Wynder, 1968 Wynder and Hoffmann, 1961
Aluminium oxide + molybdenum trioxide	⇒	Catalyst				
Aluminium oxide hydrate	3	M 24, 25				Eicher and Müller, 1985
Aluminium oxide trihydrate					S	Wynder and Hoffmann, 1961
Aluminium silicate	6, 8				S	Wynder and Hoffmann, 1961
Aluminium sulfate	3	S				Baldry <i>et al.</i> , 1988
Aluminium trihydrate	3	M 2				Armbrust and Carithers, 1968
Ambergris tincture	1	M 63		M 63		Carmines, 2002 ^c
Ambroxide	1	M 38				Miranda <i>et al.</i> , 1999
γ-Aminobutyric acid	1	S				Kaburaki <i>et al.</i> , 1969
Ammonium ceric sulfate	9	S				Bentley and Burgan, 1960
Ammonium chromic sulfate	9	S				Bentley and Burgan, 1960
Ammonium citrate	1, 3, 6	M 19–24				Eicher and Müller, 1985
Ammonium cobalt sulfate	9	S				Bentley and Burgan, 1960
Ammonium compounds	1, 3, 6	S				Ellis <i>et al.</i> , 1999
Ammonium ferric sulfate	9	S				Bentley and Burgan, 1960
Ammonium ferrous sulfate	9	S				Bentley and Burgan, 1960
Ammonium hexachloropalladate	9	S				Bryant <i>et al.</i> , 1979
Ammonium hydrogen carbonate	1, 3	S				Burton and Benner, 1972
Ammonium hydroxide	1, 3, 8	S				Stedman <i>et al.</i> , 1969
Ammonium iron(III) citrate	1, 3	M 19–24				Eicher and Müller, 1985
Ammonium iron(III) oxalate	9	M 26				Eicher and Müller, 1985

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Ammonium molybdate	9	S				Bentley and Burgan, 1960
Ammonium nickel sulfate	9	S				Bentley and Burgan, 1960
Ammonium perchlorate	9	S				Bentley and Burgan, 1960
Ammonium phosphate	3, 8	S				Grant, 1980 Halter and Ito, 1972
Ammonium sulfamate	9	S			S	Alvord and Cardon, 1956 Bentley and Burgan, 1960 Bock <i>et al.</i> , 1974 Candeli <i>et al.</i> , 1960 Cuzin <i>et al.</i> , 1960 Hoffmann and Wynder, 1968 Lindsey <i>et al.</i> , 1959 Michelson and Rathkamp, 1974 Pyriki <i>et al.</i> , 1965
Ammonium tetrachloropalladate	9	S				Bryant <i>et al.</i> , 1979
Ammonium vanadate	9	S				Burton and Benner, 1972 Burdick <i>et al.</i> , 1969 Burton, 1969
Amyl butyrate	1	M 63		M 63		Carmines, 2002 ^c
Amyl formate	1	M 63		M 63		Carmines, 2002 ^c
Amyl octanoate	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Amyris oil	1	M 63		M 63		Carmines, 2002 ^c
Anethole	1	S				Badgett and Osmalov, 1971 Bavley and Robb, 1969 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Robb <i>et al.</i> , 1964 Van Auken <i>et al.</i> , 1979
		S	S	M 61 M 60		
Angelica root oil	1	M 63		M 63		Carmines, 2002 ^c
Aniline	1, 9	S				Bentley and Burgan, 1960
Anisaldehyde	1	S				Green <i>et al.</i> , 1989 Stotesbury <i>et al.</i> , 1999 Stotesbury <i>et al.</i> , 2000 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
(<i>p</i> -Methoxy-benzaldehyde)	1	S		M 61 M 60		
		M 62, 63		M 62, 63		
Anisole	1	S M 38 S				Green <i>et al.</i> , 1989 Miranda <i>et al.</i> , 1999 Stotesbury <i>et al.</i> , 1999
Anisyl acetate	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Anisyl alcohol	1	M 63		M 63		Carmines, 2002 ^c
Anisyl formate	1	M 63		M 63		Carmines, 2002 ^c
Anisyl phenylacetate	1	M 63		M 63		Carmines, 2002 ^c
Anthracene	9	S				Thornton and Valentine, 1968
Apple juice	1			M 61		Gaworski <i>et al.</i> , 1998
Apple juice concentrate	1	M 62		M 60 M 62		Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Apricot extract	1	M 62		M 62		Carmines, 2002 ^c
L-Arginine	1			M 61		Gaworski <i>et al.</i> , 1998
Asbestos	9	M 2				Armbrust and Carithers, 1968
Ascorbic acid	1, 5	S M 51 M 52				Bentley and Burgan, 1960 Ogawa, 1998 Ohshiro, 1999
Aspartic acid	1	S		M 61		Kaburaki <i>et al.</i> , 1969 Gaworski <i>et al.</i> , 1998

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Azo-bis-isobutyronitrile	9	S				Burton and Benner, 1972
Azo-bis-isobutyronitrile (Vazo)	9	S				Terrell and Schmeltz, 1970
Balsam oil peru	1	M 63		M 63		Carmines, 2002 ^c
Balsam peru	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Barium acetate	9	S				Burton and Benner, 1972
Beeswax	1			M 61		Gaworski <i>et al.</i> , 1998
Beeswax white	1			M 60		Gaworski <i>et al.</i> , 1999a
Beet juice	1			M 61		Gaworski <i>et al.</i> , 1998
Beet juice concentrate	1			M 60		Gaworski <i>et al.</i> , 1999a
Benzaldehyde	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Green <i>et al.</i> , 1989 Miranda <i>et al.</i> , 1999 Carmines, 2002 ^c Stotesbury <i>et al.</i> , 1999
		S M 38 M 62, 63 S		M 62, 63		
Benzoic acid	1, 5		S			Kröller, 1970
Benzoin	1			M 61		Gaworski <i>et al.</i> , 1998
Benzoin resin	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Benzoin, resinoid	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Benzophenone	1	M 63		M 63		Carmines, 2002 ^c
Benzoquinone	9	S				Lakritz <i>et al.</i> , 1972
Benzothiazyl disulfide	9	S				Terrell and Schmeltz, 1970
Benzo[a]pyrene	9	S				Thornton and Valentine, 1968
Benzyl alcohol	1, 8			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
		M 62, 63		M 62, 63		
Benzyl benzoate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Benzyl butyrate	1	M 63		M 63		Carmines, 2002 ^c
Benzyl cinnamate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Benzyl propionate	1	M 63		M 63		Carmines, 2002 ^c
Benzyl salicylate	1	M 63		M 63		Carmines, 2002 ^c
Bergamot oil	1	M 63		M 63		Carmines, 2002 ^c
Bisabolene	1	M 63		M 63		Carmines, 2002 ^c
Bismuth oxide	9	S				Chakraborty <i>et al.</i> , 1971
Bois de rose oil	1	M 63		M 63		Carmines, 2002 ^c
Borate	5	S S S S				Benner <i>et al.</i> , 1969a, Benner <i>et al.</i> , 1969b Burdick <i>et al.</i> , 1969 Burton, 1969
Boric acid	3, 5	S			S	Burton and Benner, 1972 Wynder and Hoffmann, 1961
Borneol	1	M 63		M 63		Carmines, 2002 ^c
Bornyl acetate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Bornyl isovalerate	1	M 63		M 63		Carmines, 2002 ^c
Brown invert syrup	1, 2			M 60		Gaworski <i>et al.</i> , 1999a
Buchu leaves oil	1	M 63		M 63		Carmines, 2002 ^c
Buckthorne berry extract	7		S			Kröller, 1963a
Butanediol ⇨ butylene glycol						
2,3-Butanedione	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Butter	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Butyl alcohol	1, 8	M 63		M 63		Carmines, 2002 ^c
Butyl butyrate	1	M 63		M 63		Carmines, 2002 ^c
Butyl butyrylactate	1	M 63		M 63		Carmines, 2002 ^c
1,3-Butylene glycol	2, 8	M 6 M 10 M 13, 14 S S	S	M 60 M 61		Carugno <i>et al.</i> , 1971 Detert and Ruchholz, 1974 Doihara <i>et al.</i> , 1964 Dontenwill <i>et al.</i> , 1972 Gaworski <i>et al.</i> , 1999a Gaworski <i>et al.</i> , 1998 Kobashi <i>et al.</i> , 1965 Kröller, 1964b Smit, 1970
2,3-Butylene glycol	2	S				Kobashi <i>et al.</i> , 1965
3-Butylidenephthalide	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Butyl 2-ethyl-3-hydroxy-3-methyl-3-toluypropionate	⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate				
Butyl isovalerate	1	M 63		M 63		Carmines, 2002 ^c
2,6-di- <i>tert.</i> Butyl- <i>v</i> -methylphenol	5, 8	S				Burton and Benner, 1972
Butyl phenylacetate	1	M 63		M 63		Carmines, 2002 ^c
Butyric acid	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Calcium alginate	6	M 53				Prouse <i>et al.</i> , 1977
Calcium carbonate	3	M 5 M 10 M 19–26 M 48, 49				Briskin, 1979 Detert and Ruchholz, 1974 Eicher and Müller, 1985 NCI, Report No. 4, 1980 Wynder and Hoffmann, 1961
Calcium ethylvanillin-5-carboxylate	⇒	5-carboxyvanillin			S	
Calcium nitrate	9	S S				Johnson <i>et al.</i> , 1973 Kallianos <i>et al.</i> , 1968
Calcium oxalate	9	S				Chakraborty <i>et al.</i> , 1971
Calcium vanillin-5-carboxylate	⇒	5-carboxyvanillin				
Campeachy wood extract	7		S			Kröller, 1963b
Camphene	1	M 62		M 62		Carmines, 2002 ^c
Cananga oil	1	M 63		M 63		Carmines, 2002 ^c
Caramel colour	1, 7			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Caraway oil	1	M 63		M 63		Carmines, 2002 ^c
Carbon	7	M 36, 37				Miano and Keith, 1976
Carbon (activated)	6	M 1				An <i>et al.</i> , 1996
Carbowax	⇒	polyethylene glycols				
5-Carboxyethylvanillin	⇒	5-Carboxyvanillin				
Carboxymethylcellulose	6	M 1 M 11 S, M 35–37	S S			An <i>et al.</i> , 1996 Dontenwill <i>et al.</i> , 1972 Kröller, 1964a Miano and Keith, 1976 Sjöberg and Pyysalo, 1985
Carboxymethyl starch	6		S			Kröller, 1966a
5-Carboxyvanillin	1		S			Southwick, 1992
Cardamom oil	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Cardamom seed oil	1	M 63		M 63		Carmines, 2002 ^c
Carob bean and extract	1, 6			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Carob (locust bean gum)	1, 6, 8		S			Sjöberg and Pyysalo, 1985
Carob seed powder	1, 6		S			Kröller, 1965b
Carrot oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
4-Carvomenthenol	1	M 63		M 63		Carmines, 2002 ^c
L-Carvone	1	M 63		M 63		Carmines, 2002 ^c
1-Carvyl 2-methyl-3-hydroxy-3-methyl-3-toluypropionate			⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate		
β-Caryophyllene	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
β-Caryophyllene oxide	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Cascarilla bark oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Casein	9		S S			Higman, E.B. <i>et al.</i> , 1970 Schmeltz <i>et al.</i> , 1972
Casein hydrolysate	9	S				Crosthwaite <i>et al.</i> , 1979
Cassia absolute	1	M 63		M 63		Carmines, 2002 ^c
Cassia bark	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Castoreum extract	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Catalyst (MoO ₃ + Al ₂ O ₃)	9	S				Terrell and Schmeltz, 1970
Celery oleoresin	1	M 63		M 63		Carmines, 2002 ^c
Celery seed oil	1	M 63		M 63		Carmines, 2002 ^c
Cellobiose	9		S			Schlotzhauer <i>et al.</i> , 1967
Cellubiose	9		S			Kato, 1967
Cellulose	6	M 5 S	S			Bell <i>et al.</i> , 1966 Briskin, 1979 Carmella <i>et al.</i> , 1984 Cullis <i>et al.</i> , 1983a Cullis <i>et al.</i> , 1983b Dontenwill <i>et al.</i> , 1976 Gilbert and Lindsey, 1957 Higman, E.B. <i>et al.</i> , 1970 Jenkins <i>et al.</i> , 1980 Kato, 1967 Kröller, 1964a NCI, Report No. 4, 1980 Prouse <i>et al.</i> , 1977 Robb <i>et al.</i> , 1966 Sakuma <i>et al.</i> , 1981 Schlotzhauer <i>et al.</i> , 1967 Schlotzhauer <i>et al.</i> , 1982 Schlotzhauer <i>et al.</i> , 1985 Wakeham and Silberman, 1966
		M 16, 17	S			
		S	S			
		S, M 48 M 53	S S	S		
		S	S			
Cellulose acetate	6	M 10				Detert and Ruchholz, 1974
Cellulose ether gums	6	M 46, 47, 49			M 46, 47	NCI, Report No. 4, 1980
Cellulose monoacetate	9		S			Kröller, 1964a
Cellulose sulfate	6	M 19–26				Eicher and Müller, 1985
Chalk	3, 6	M 31–34				McAdam, 1997
Chamomile, flower, Hungarian, oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Chamomile, flower, Roman, extract	1	M 63		M 63		Carmines, 2002 ^c
Chamomile, flower, Roman, oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Chamomile flower oil	1			M 60		Gaworski <i>et al.</i> , 1999a
Chamomile oil	1			M 61		Gaworski <i>et al.</i> , 1998

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Chamomile oil, German	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Chemosol	9				M 65	Gargus <i>et al.</i> , 1975
Chicory extract	1	M 62		M 62		Carmines, 2002 ^c
Chlorogenic acid	9	S	S			Carmella <i>et al.</i> , 1984 Schlotzhauer <i>et al.</i> , 1982
Chlorophyll	1	M 28 M 52				Komatsu, 1997 Ohshiro, 1999
Chlorophyllin	9	S				Crosthwaite <i>et al.</i> , 1979
Chocolate	1	M 63		M 63		Carmines, 2002 ^c
Cholesterol	9	S				Cheng, 1973
Cineol	1	S				Bavley and Robb, 1969
Cinnamaldehyde	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cinnamic acid	1	M 63		M 63		Carmines, 2002 ^c
Cinnamon bark oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cinnamon leaf oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cinnamyl acetate	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Cinnamyl alcohol	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Cinnamyl cinnamate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cinnamyl 2-isopropyl-3-hydroxy-3-methyl-3-toluypropionate		M 62, 63		M 62, 63		Carmines, 2002 ^c
Cinnamyl isovalerate	1	S M 63	⇒			Mathis, 1983 Carmines, 2002 ^c
Cinnamyl propionate	1	S				Mathis, 1983
Citral	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Citric acid	1, 3, 5	M 62 M 11, 12 M 18		M 62 S		Carmines, 2002 ^c Dalhamn and Rylander, 1971 Dontenwill <i>et al.</i> , 1972 Dontenwill <i>et al.</i> , 1976 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Gilbert and Lindsey, 1957 Kröller, 1966b NCI, Report No. 4, 1980 Ogawa, 1998 Stedman <i>et al.</i> , 1969
			S S			
		M 47 M 51 S			M 47	
Citronellal	1	S				Bavley and Robb, 1969
Citronella oil	1	M 63		M 63		Carmines, 2002 ^c
Citronellol (Rhodinol)	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
D,L-Citronellol	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Citronellyl isobutyrate	1	M 63		M 63		Carmines, 2002 ^c
Citron oil	1	S				Bavley and Robb, 1969
Citrus fruit or herb	1	M 52				Ohshiro, 1999
Civet absolute	1	M 63		M 63		Carmines, 2002 ^c
Clary oil	1	M 63		M 63		Carmines, 2002 ^c
Clay	3, 8	M 48				NCI, Report No. 4, 1980
Cobalt (III) oxide	9				S	Wynder and Hoffmann, 1961
Cocoa	1	M 31–34 S		S S		McAdam, 1997 NCI, Report No. 3, 1977
(Cacao)		M 63	S	M 63		Römer and Hackenberg, 1990 Carmines, 2002 ^c Schlotzhauer, 1978
Cocoa extract	1			M 61 M 62, 63		Gaworski <i>et al.</i> , 1998 Carmines, 2002 ^c
Cocoa powder	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Cocoa shell extract	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cocoa shells	1	M 64		M 64		Carmines, 2002 ^c
Coffee	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Coffee extract	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cognac	1			M 61		Gaworski <i>et al.</i> , 1998
Cognac, green, oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Cognac, white	1			M 60		Gaworski <i>et al.</i> , 1999a
Collagen	9		S S			Higman, E.B. <i>et al.</i> , 1970 Schmeltz <i>et al.</i> , 1972
Colorant	7	M 36, 37				Miano and Keith, 1976
Comfrey powder	1	M 51				Ogawa, 1998
Copaiba oil	1	M 63		M 63		Carmines, 2002 ^c
Copper nitrate	9	S			S S S S	Bentley and Borgan, 1960 Hoffmann and Wynder, 1968 Wynder and Hoffmann, 1961 Wynder and Hoffmann, 1963 Wynder and Hoffmann, 1969
Copper sulfate	9	S				Bentley and Borgan, 1960
Coriander oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Corn silk	1	M 62		M 62		Carmines, 2002 ^c
Costus root oil	1	M 63		M 63		Carmines, 2002 ^c
<i>o</i> -, <i>m</i> -, <i>p</i> -Cresol	1	S				Bavley and Robb, 1969
Cubeb oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Coumarin	1	S				Bavley and Robb, 1969
Cyclodextrins	1, 5, 6		S			Robb <i>et al.</i> , 1964
Cyclohexanone	1, 7, 8	S				Bavley and Robb, 1969
Cyclohexyl 3-hydroxy-3-methyloctanoate	⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate				
Cyclopentadiene	1		S			Robb <i>et al.</i> , 1964
<i>p</i> -Cymene	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
<i>p</i> -Cymol	1	S				Bavley and Robb, 1969
β-Damascenone	1	S M 38				Jing and Xian, 1999 Miranda <i>et al.</i> , 1999
β-Damascone	1	S		M 61		Jing and Xian, 1999 Gaworski <i>et al.</i> , 1998
Dandelion root extract solid	1	M 62		M 62		Carmines, 2002 ^c
Davana oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
γ-Decalactone	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
δ-Decalactone	1	M 63		M 63		Carmines, 2002 ^c
Decanal	1	M 63		M 63		Carmines, 2002 ^c
Decanoic acid	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
1-Decanol	1, 8	M 58 M 62		M 58 M 62		Tso, 1975 Carmines, 2002 ^c
Deertongue leaf powder	1		S			Higman, H.C. <i>et al.</i> , 1974
<i>endo</i> -Dehydronorborneol	1		S			Robb <i>et al.</i> , 1964
Dextrin	1, 6		S			Schlotzhauer <i>et al.</i> , 1985
Diacetyl	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Dialdehyde crosslinker	6	M 46, 47, 49			M 46, 47	NCI, Report No. 4, 1980

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Dialdehyde starch (Oxystarch)	6		S			Kröller, 1966a
Diammonium palladiumnitrite	9	S				Bryant <i>et al.</i> , 1979
Diammonium phosphate	1, 3, 6, 8	M 62 S M 54		M 62 S		Carmines, 2002 ^c Mariner <i>et al.</i> , 2000 Saint-Jalm <i>et al.</i> , 2000 Misra <i>et al.</i> , 2001
Diammonium platininitrite	9	S				Bryant <i>et al.</i> , 1979
Dibutyl phthalate	4		S			Kröller, 1968
Diethylamine	1	S				Stedman <i>et al.</i> , 1969
Diethylamine citrate	9				S	Dalhamn and Rylander, 1971
Diethylene glycol	2	S M 6 M 12, 15 M 16–18 S S	S			Aksu, 1969 Carugno <i>et al.</i> , 1971 Dontenwill <i>et al.</i> , 1972 Dontenwill <i>et al.</i> , 1976 Kratchanova <i>et al.</i> , 1995 Kröller, 1964b Stoilova <i>et al.</i> , 1994
2,3-Diethylpyrazine	1	M 63		M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Diethyl sebacate	1, 4	M 62		M 62		Carmines, 2002 ^c
Dill oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
<i>m</i> -Dimethoxybenzene	1	M 63		M 63		Carmines, 2002 ^c
<i>p</i> -Dimethoxybenzene	1	M 63		M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2,4-Dimethylacetophenone	1	M 62		M 62		Carmines, 2002 ^c
3,4-Dimethyl-1,2-cyclopentanedione	1			M 61		Gaworski <i>et al.</i> , 1998
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
3,7-Dimethyl-1,3,6-octatriene	1	M 62		M 62		Carmines, 2002 ^c
3,7-Dimethyl-1,6-octadiene-3-ol	1			M 60		Gaworski <i>et al.</i> , 1999a
3,7-Dimethyl-6-octenoic acid	1	M 63		M 63		Carmines, 2002 ^c
α,α -Dimethylphenethyl acetate	1	M 62		M 62		Carmines, 2002 ^c
α,α -Dimethylphenethyl butyrate	1	M 62		M 62		Carmines, 2002 ^c
2,3-Dimethylpyrazine	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
2,5-Dimethylpyrazine	1	M 63		M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2,6-Dimethylpyrazine	1			M 60		Gaworski <i>et al.</i> , 1999a
Dimethyltetrahydro-benzo-furanone	1	M 62		M 62		Carmines, 2002 ^c
6,10-Dimethyl-5,9-undecadien-2-one	1	M 62		M 62		Carmines, 2002 ^c
Dipropylamine	9	S S				Lakritz <i>et al.</i> , 1969 Stedman <i>et al.</i> , 1969
Disodium carbonate	3, 6	S				Stedman <i>et al.</i> , 1969
Disodium hydrogen phosphate	3, 8	S M 5				Baldry <i>et al.</i> , 1988 Briskin, 1979
Docosane	1		S			Bell <i>et al.</i> , 1966
γ -Dodecalactone	1	M 63		M 63		Carmines, 2002 ^c
δ -Dodecalactone	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Dolomitic limestone	6	S, M 35–37				Miano and Keith, 1976
Dotriacontane	9	S S				Jenkins <i>et al.</i> , 1970a Jenkins <i>et al.</i> , 1973
Estragole	1	M 38				Miranda <i>et al.</i> , 1999
4-Ethoxyacetophenone	1	S				Mathis, 1972
Ethyl acetate	1, 8			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl acetoacetate	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Ethyl alcohol	1, 8			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl benzoate	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl 2-(2-butyl)-3-hydroxy-3-methyldodecanoate		⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate			
Ethyl 2-(2-butyl)-3-hydroxy-3-methylnonanoate		⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate			
Ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate	1		S			Grubbs and Houminer, 1982
Ethyl butyrate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Ethyl- <i>n</i> -caprylate	1	S				Bavley and Robb, 1969
Ethylcellulose	6	S				Halter and Ito, 1972
Ethyl cinnamate	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl decanoate	1			M 61 M 63		Gaworski <i>et al.</i> , 1998 Carmines, 2002 ^c
2-Ethyl-3(5 or 6)-dimethylpyrazine	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethylene glycol	2, 8	S S S S				Bentley and Burgan, 1960 Bilimoria and Nisbet, 1975 Pyriki <i>et al.</i> , 1965 Reif, 1949
Ethyl heptanoate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Ethyl hexanoate	1			M 61 M 62, 63		Gaworski <i>et al.</i> , 1998 Carmines, 2002 ^c
Ethylhydroxyethyl cellulose	6	M 40			M 40	NCI, Report No. 1, 1976
5-Ethyl-3-hydroxy-4-methyl-2(5 <i>H</i>)-furanone	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl 2-isopropyl-3-hydroxy-3-methyl-3-phenylpropionate		⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate			
Ethyl isovalerate	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl lactate	1, 8			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl laurate	1			M 61 M 63		Gaworski <i>et al.</i> , 1998 Carmines, 2002 ^c
Ethyl levulinate	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Ethyl maltol	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2-Ethyl (or Me)-(3,5 and 6)-methoxypyrazine	1			M 61		Gaworski <i>et al.</i> , 1998

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Ethyl 2-methylbutyrate	1	M 62		M 62		Carmines, 2002 ^c
2-Ethyl-3-methylpyrazine	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl myristate	1			M 61		Gaworski <i>et al.</i> , 1998
Ethyl nonanoate	1	M 63		M 63		Carmines, 2002 ^c
Ethyl octanoate	1			M 61		Gaworski <i>et al.</i> , 1998
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Ethyl palmitate	1			M 61		Gaworski <i>et al.</i> , 1998
Ethyl phenylacetate	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl propionate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Ethyl 2-propyl-3-hydroxy-3-methyl-3-phenylpropionate		⇒		ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate		
Ethyl 2-propyl-3-hydroxy-3-phenylpropionate		⇒		ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate		
3-Ethylpyridine	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Ethyl valerate	1	M 30				Matsushita and Shinozaki, 1980
Ethyl vanillin	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ethyl vanillyl-D-glucoside	⇒	4-(β-D-glucopyranosyloxy)-3-ethoxybenzaldehyde				
Eucalyptol	1	M 63		M 63		Carmines, 2002 ^c
Eugenol	1	S				Burton and Benner, 1972
Farnesol	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
FD & C 1956 Brown	7	M 53				Prouse <i>et al.</i> , 1977
Fenugreek/fenugreek extract	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Ferric ammonium citrate	⇒	ammonium iron(III) citrate				
Ferric ammonium oxalate	⇒	ammonium iron(III) oxalate				
Fibre	6	M 3				Biggs <i>et al.</i> , 1998
Fig juice/fig juice concentrate	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Flavour C 146	1	M 53				Prouse <i>et al.</i> , 1977
Flavour mixture (brown, aromatic taste)	1		S			Kröller, 1967
Food starch, modified	6			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Formic acid	1	S S				Lakritz <i>et al.</i> , 1969 Stedman <i>et al.</i> , 1969
Fructose	1	S S				Burton and Benner, 1972 Carmella <i>et al.</i> , 1984 Gilbert and Lindsey, 1957 Higman, E.B. <i>et al.</i> , 1970 Schlotzhauer <i>et al.</i> , 1982 Thornton and Massey, 1975
		S, M 56				
Furan	1		S			Robb <i>et al.</i> , 1964
Furan-acetylene-dicarboxylic acid	1	S				Robb <i>et al.</i> , 1964
Furfuryl 3-hydroxy-3-ethyltredecanoate	⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate				
Furfuryl mercaptan	1			M 61		Gaworski <i>et al.</i> , 1998
4-(2-Furyl)-3-butene-2-one	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Gaballon	1	M 28				Komatsu, 1997
Galacto-mannan gums	6	M 46, 47, 49			M 46, 47	NCI, Report No. 4, 1980
Galbanum oil	1	M 63		M 63		Carmines, 2002 ^c
Gallic acid	9	S				Burton and Benner, 1972
Galvinoxyl	9	S				Burton and Benner, 1972
Genet absolute	1	M 63		M 63		Carmines, 2002 ^c
Geraniol	1, 9	S M 62, 63		M 62, 63		Bavley and Robb, 1969 Carmines, 2002 ^c
Geranium rose oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Geranyl acetate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Geranyl acetone	1	S				Jing and Xian, 1999
Geranyl butyrate	1	M 63		M 63		Carmines, 2002 ^c
Geranyl formate	1	M 63		M 63		Carmines, 2002 ^c
Geranyl 3-hydroxy-3-methyloctanoate	⇒	ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate				
Geranyl phenylacetate	1	M 62		M 62		Carmines, 2002 ^c
Ginger oil	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
4-(β-D-glucopyranosyloxy)-3-ethoxybenzaldehyde	1		S			Herron, 1988
Glucose	1	S S S S S, M 56 S	S S S S S			Bell <i>et al.</i> , 1966 Crosthwaite <i>et al.</i> , 1979 Gager <i>et al.</i> , 1971a Gager <i>et al.</i> , 1971b Gilbert and Lindsey, 1957 Higman, E.B. <i>et al.</i> , 1970 Kato, 1967 Schlotzhauer <i>et al.</i> , 1967 Thornton and Massey, 1975 Thornton and Valentine, 1968 Tomasik, 1989 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Glucuronic acid	9		S			Schlotzhauer <i>et al.</i> , 1967
Glutamic acid	1	S				Kaburaki <i>et al.</i> , 1969
Glycerol	2	M 1 M 2 S M 3 S, M 4 M 5 M 6 S M 10				An <i>et al.</i> , 1996 Armbrust and Carithers, 1968 Bentley and Burgan, 1960 Biggs <i>et al.</i> , 1998 Bilimoria and Nisbet, 1975 Briskin, 1979 Carugno <i>et al.</i> , 1971 De Souza and Scherbak, 1964 Detert and Ruchholz, 1974 Doihara <i>et al.</i> , 1964 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Gaworski <i>et al.</i> , 1999b Ishiguro <i>et al.</i> , 1979 Jenkins <i>et al.</i> , 1980 Kobashi <i>et al.</i> , 1965 Kröller, 1965a Laurene <i>et al.</i> , 1965 Cook <i>et al.</i> , 1999 McAdam, 1997 NCI, Report No. 3, 1977 Pyriki <i>et al.</i> , 1965 Carmines, 2002 ^c Settle <i>et al.</i> , 1999 Smit, 1970 Stein and Antal, 1983 Stoilova <i>et al.</i> , 1994
			S	M 61 M 60 S, M 59		
		S S S S S M 31–34 S, M 41–44 S M 62, 63 M 55 S			S M 62, 63	
		S	S			
Glyceryl monoacetate (monoacetin)	4, 6		S			Kröller, 1968

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Glycine	1	S	S			Johnson <i>et al.</i> , 1973 Schmeltz <i>et al.</i> , 1972
Glycosylamine	1	S				Cox <i>et al.</i> , 1987
Glycyrrhetic acid	1	S				Sakagami, 1973
Glycyrrhizae radix	1	M 51				Ogawa, 1998
Glycyrrhizic acid	1	S	S			Sakagami, 1973 Yongkuan and Wangyun, 1995
Glycyrrhizic acid disodium salt	1		S			Yongkuan and Wangyun, 1995
Glycyrrhizic acid monosodium salt	1		S			Yongkuan and Wangyun, 1995
Glycyrrhizic acid trisodium salt	1		S			Yongkuan and Wangyun, 1995
Glyoxal	5, 6	M 12 M 18	S			Dontenwill <i>et al.</i> , 1972 Dontenwill <i>et al.</i> , 1976 Kröller, 1970
Guaiac wood oil	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Guaiacol	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Guar (oxygenated)	6		S			Kröller, 1968
Guar gum	6	M 2	S S			Armbrust and Carithers, 1968 Kröller, 1965b Sjöberg and Pyysalo, 1985
Gummi arabicum	6		S S			Kröller, 1965b Sjöberg and Pyysalo, 1985
2,4-Heptadienal	1	M 63		M 63		Carmines, 2002 ^c
γ-Heptalactone	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Heptanoic acid	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
2-Heptanone	1	M 63		M 63		Carmines, 2002 ^c
3-Hepten-2-one	1	M 62		M 62		Carmines, 2002 ^c
ω-6-Hexadecenlactone	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Hexadien-(2,4)-al	1	S				Bavley and Robb, 1969
γ-Hexalactone	1			M 61 M 60 M 62		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Hexanal	1	M 63		M 63		Carmines, 2002 ^c
Hexanoic acid	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Hexen-2-al	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
trans-2-Hexenoic acid	1	M 62		M 62		Carmines, 2002 ^c
3-Hexen-1-ol	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Hexyl acetate	1	M 63		M 63		Carmines, 2002 ^c
Hexyl 2-methylbutanoate	1	M 63		M 63		Carmines, 2002 ^c
Hexyl phenylacetate	1	M 63		M 63		Carmines, 2002 ^c
Honey	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Humectant	2	M 51				Ogawa, 1998
Humic acid, sodium salt	7		S			Kröller, 1963c
p-Hydroxybenzoic acid ethylester	5		S			Kröller, 1970
4-Hydroxy-2,5-dimethyl-3(2H)-furanone	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Hydroxyethyl cellulose	6		S			Kröller, 1964a
4-(<i>p</i> -Hydroxyphenyl)-2-butanone	1			M 61 M 60 M 62		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Hyssop oil	1	M 63		M 63		Carmines, 2002 ^c
Hz-1 catalyst	9	S				Terrell and Schmeltz, 1970
Immortelle	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Immortelle extract	1	M 63		M 63		Carmines, 2002 ^c
Indole	1	S				Burton and Benner, 1972
Inositol	2	M 5				Briskin, 1979
Invert sugar ⇒ sugar						
Ionone	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
α-Ionone	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
β-Ionone	1	S				Jing and Xian, 1999
Iron(III) chloride	3, 6, 7, 9	M 26				Eicher and Müller, 1985
Iron(III) oxide hydrate	7	M 21–24				Eicher and Müller, 1985
Isoamyl acetate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Isoamyl benzoate	1	S M 63		M 63		Mathis, 1983 Carmines, 2002 ^c
Isoamyl butyrate	1	M 63		M 63		Carmines, 2002 ^c
Isoamyl cinnamate	1	S M 63		M 63		Mathis, 1983 Carmines, 2002 ^c
Isoamyl formate	1	M 63		M 63		Carmines, 2002 ^c
Isoamyl hexanoate	1	M 63		M 63		Carmines, 2002 ^c
Isoamyl isovalerate	1	S S S M 63		M 63		Green <i>et al.</i> , 1989 Mathis, 1983 Stotesbury <i>et al.</i> , 1999 Carmines, 2002 ^c
Isoamyl phenylacetate	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Mathis, 1983 Carmines, 2002 ^c
Isoamyl salicylate	1	M 62		M 62		Carmines, 2002 ^c
Isobutyl acetate	1	M 63		M 63		Carmines, 2002 ^c
Isobutyl alcohol	1, 6, 7	M 62, 63		M 62, 63		Carmines, 2002 ^c
Isobutyl cinnamate	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2-Isobutyl-3-methoxypyrazine	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
α-Isobutylphenethyl alcohol	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Isobutyl phenylacetate	1	M 63		M 61 M 63		Gaworski <i>et al.</i> , 1998 Carmines, 2002 ^c
Isobutyraldehyde	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Isobutyric acid	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Isoeugenol	1		S			Schlotzhauer <i>et al.</i> , 1967
Isoprene	1		S			Robb <i>et al.</i> , 1964 Van Auken <i>et al.</i> , 1979

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Isovaleric acid	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Jasmine absolute	1	M 63		M 63		Carmines, 2002 ^c
Kola nut extract	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Labdanum absolute	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62		M 62		Carmines, 2002 ^c
Lactic acid	1	S		M 61 M 60		Lakritz <i>et al.</i> , 1969 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
			S			Kröller, 1966b
Lactose	1, 9		S			Tomasik, 1989
Lauric acid	1	M 63		M 63		Carmines, 2002 ^c
Lavender oil	1	M 63		M 63		Carmines, 2002 ^c
Lead borate	9	S				Terrell and Schmeltz, 1970
Lead nitrate	9	S				Bentley and Burgan, 1960
Lemongrass oil	1	M 63		M 63		Carmines, 2002 ^c
Lemon oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Lemon oil terpenes	1	M 63		M 63		Carmines, 2002 ^c
Lettuce leaves	1		S			Kröller, 1970
Licorice	1		S			Chung and Aldridge, 1999
			S			Fratini <i>et al.</i> , 1977
			S	M 61		Gaworski <i>et al.</i> , 1998
		M 31–34				Kröller, 1967
						McAdam, 1997
Licorice extract	1, 7			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62,64		M 62, 64		Carmines, 2002 ^c
Lignin	9		S			Gilbert and Lindsey, 1957
			S			Schlotzhauer <i>et al.</i> , 1967
			S			Schlotzhauer <i>et al.</i> , 1982
			S			Schlotzhauer <i>et al.</i> , 1985
Lime oil	1	M 63		M 63		Carmines, 2002 ^c
Lime oil, terpeneless	1	M 63		M 63		Carmines, 2002 ^c
<i>d</i> -Limonene	1	S				Bavley and Robb, 1969
Linalool	1	S				Bavley and Robb, 1969
				M 61 M 63		Gaworski <i>et al.</i> , 1998
		M 63		M 63		Carmines, 2002 ^c
Linalyl acetate	1	M 63		M 63		Carmines, 2002 ^c
Lithium nitrate	9	S				Burton and Benner, 1972
Lovage extract	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Lovage oil	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Lycopodium bisdepuratum (seeds of club moss)	9	M 29				Kossack, 1987
L-Lysine	1			M 61		Gaworski <i>et al.</i> , 1998
Mace oil	1	M 63		M 63		Carmines, 2002 ^c
Madder lake	7		S			Kröller, 1963d
Magnesium acetate	3, 6	S				Aksu, 1969
Magnesium aluminium citrate	3	M 25				Eicher and Müller, 1985
Magnesium carbonate	3, 6, 7	S				Burton and Benner, 1972
		S				Terrell and Schmeltz, 1970
Magnesium iron(III) citrate	3	M 19–24				Eicher and Müller, 1985

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Magnesium nitrate	9	S, M 7–9 S, M 42, 44, 45 S, M 50			S S, M 45	Collins <i>et al.</i> , 1981 Kier <i>et al.</i> , 1974 NCI, Report No. 3, 1977 Norman and Bryant, 1975
Magnesium oxide	3, 6, 7				S	Wynder and Hoffmann, 1961
Magnesium vanillin-5-carboxylate	⇒	5-carboxyvanillin				
Maleic anhydride	9	S				Thornton and Valentine, 1968
Malic acid	1		S	M 61		Kröller, 1966b Gaworski <i>et al.</i> , 1998 Gilbert and Lindsey, 1957
Malt	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Malt extract	1	M 62		M 62		Carmines, 2002 ^c
Maltodextrin	1, 6			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Maltol	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Maltose	1	M 51				Ogawa, 1998 (Patent)
Mandarin oil	1	M 63		M 63		Carmines, 2002 ^c
Manganese iron(III) citrate	9	M 19–24				Eicher and Müller, 1985
Manganese nitrate	9	S				Burton and Benner, 1972
Maple syrup	1	M 62		M 62		Carmines, 2002 ^c
Mate absolute	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Mate leaf	1			M 61		Gaworski <i>et al.</i> , 1998
Megastigmatrienone	1	S				Yang <i>et al.</i> , 2001
Melamine-formaldehyde resin	6		S			Kröller, 1968
Melilot	1		S			Kröller, 1967
Menthol	1	S S S S M 63, 64 S S S S M 30 M 38 S S S S S M 55 S M 57		S M 63, 64 S M 61 M 60		Badgett and Osmalov, 1971 Bavley and Robb, 1969 BAT Co Ltd., 1978 Bombick <i>et al.</i> , 2001 Brozinski <i>et al.</i> , 1972 Carmines, 2002 ^c Curran, 1972 Curran, 1975 Gaworski <i>et al.</i> , 1997 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Grubbs <i>et al.</i> , 1978 Jenkins <i>et al.</i> , 1970b Jing and Xian, 1999 Cook <i>et al.</i> , 1999 Lyerly, 1967 Matsushita and Shinozaki, 1980 Miranda <i>et al.</i> , 1999 Mitchell <i>et al.</i> , 1963 Nichols <i>et al.</i> , 1987 Perfetti and Gordin, 1985 Rakieten <i>et al.</i> , 1952 Riehl <i>et al.</i> , 1973 Robb <i>et al.</i> , 1964 Schmeltz and Schlotzhauer, 1968 Settle <i>et al.</i> , 1999 Shepherd and Gould, 1968 Tiggelbeck and Manes, 1976 Van Duuren <i>et al.</i> , 1968
Menthone	1	S		M 61 M 60 M 62		Bavley and Robb, 1969 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Methanol	9	M 10				Detert and Ruchholz, 1974
Methocel	⇒	methylcellulose				

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Methofuran	1		S			Robb <i>et al.</i> , 1964
<i>p</i> -Methoxybenzaldehyde	⇒	anisaldehyde				
2-Methoxy-4-methylphenol	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2-Methoxy-3-methylpyrazine	1	M 63		M 63		Carmines, 2002 ^c
Methoxymethylthiirane	9	S				Burton and Benner, 1972
1-Methoxy-(4-(2-propenyl)benzene	⇒	Estragole				
Methoxypyrazine	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
4'-Methylacetophenone	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Methyl anthranilate	1	M 63		M 63		Carmines, 2002 ^c
Methyl benzoate	1	S				Mathis, 1983
3-Methylbutyraldehyde	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2-Methylbutyric acid	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Methyl caprate	1	S			S	Tso, 1975
Methyl cellulose	6, 9	M 10 M 13, 14				Detert and Ruchholz, 1974 Dontenwill <i>et al.</i> , 1972 Kröller, 1964a
(Methocel)		M 40	S		M 40	NCI, Report No.1, 1976
Methyl cinnamate	1	S S M 62 S		M 62		Green <i>et al.</i> , 1989 Mathis, 1983 Carmines, 2002 ^c Stotesbury <i>et al.</i> , 1999
Methylcyclopentenolone	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Methyl 2,2-dimethyl-3-hydroxy-3-methyl-3-phenylpropionate	⇒					ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate
Methyl 2,2-dimethyl-3-hydroxy-3-phenylpropionate	⇒					ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate
Methylene chloride	9	M 10				Detert and Ruchholz, 1974
6-Methyl-3,5-heptadien-2-one	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2-Methylheptanoic acid	1			M 61		Gaworski <i>et al.</i> , 1998
6-Methyl-5-hepten-2-one	1	M 63		M 63		Carmines, 2002 ^c
2-Methylhexanoic acid	1	M 63		M 63		Carmines, 2002 ^c
Methyl isovalerate	1	M 63		M 63		Carmines, 2002 ^c
Methyl linoleate	1	M 63		M 63		Carmines, 2002 ^c
Methyl linolenate	1	M 63		M 63		Carmines, 2002 ^c
2-Methyl-(3,5 and 6)-methoxypyrazine	⇒	2-ethyl (or Me)-(3,5 and 6)-methoxypyrazine				
Methyl phenylacetate	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
5-Methyl-2-phenyl-2-hexenal	1	M 63		M 63		Carmines, 2002 ^c
2-Methylpyrazine	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Methyl salicylate	1	S M 63		M 63		Bavley and Robb, 1969 Carmines, 2002 ^c
Methyl starch	6		S			Kröller, 1966a
2-Methyl-tetrahydrofuran-3-one	1	M 63		M 63		Carmines, 2002 ^c
2-Methylvaleric acid	1	M 62		M 62		Carmines, 2002 ^c
Mica	7	M 10				Detert and Ruchholz, 1974
Mimosa	1	M 62, 63		M 62, 63		Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Molasses, blackstrap	1	M 62		M 62		Carmines, 2002 ^c
Molybdenum trioxide + aluminium oxide	⇒	Catalyst				
Momordica grosvenori	9	M 28				Komatsu, 1997
Monoacetin ⇒ glyceryl monoacetate						
Mountain maple solid extract	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Myrcene	1	S	S			Bavley and Robb, 1969 Robb <i>et al.</i> , 1964
Myrrh oil	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Neophytadiene	1	S				Schmeltz <i>et al.</i> , 1978
Nerol	1	M 62		M 62		Carmines, 2002 ^c
Neroli bigarade oil	1	M 63		M 63		Carmines, 2002 ^c
Nickel acetate	9	S			S	Wynder and Hoffmann, 1963 Hoffmann and Wynder, 1968
Nickel oxalate	9	S				Terrell and Schmeltz, 1970
Nitrate	9				S S	Dontenwill <i>et al.</i> , 1976 Collins <i>et al.</i> , 1981
N-Nitrosodimethylamine	9	S				Morie and Sloan, 1973
Nona-2- <i>trans</i> , 6- <i>cis</i> -dienal	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
γ-Nonalactone	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Nonanal	1	M 63		M 63		Carmines, 2002 ^c
Nonanoic acid	1	M 63		M 63		Carmines, 2002 ^c
<i>trans</i> -2-Nonen-1-ol	1	M 63		M 63		Carmines, 2002 ^c
Nonyl acetate	1	M 63		M 63		Carmines, 2002 ^c
Nutmeg oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Oak moss	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
γ-Octalactone	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
δ-Octalactone	1	M 63		M 63		Carmines, 2002 ^c
Octanal	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
<i>n</i> -Octane	1, 8	S				Bavley and Robb, 1969
Octanoic acid	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
		M 63				
1-Octanol	1, 8	M 58		M 58		Tso, 1975
1-Octen-3-ol	1			M 60 M 61		Gaworski <i>et al.</i> , 1999a Gaworski <i>et al.</i> , 1998
1-Octen-3-yl acetate	1	M 62		M 62		Carmines, 2002 ^c
Octyl isobutyrate	1	M 63		M 63		Carmines, 2002 ^c
Opoponax gum	1	M 63		M 63		Carmines, 2002 ^c
Opoponax oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Orange oil and products		S				Bavley and Robb, 1969
	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Orange oil terpenes	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Origanum oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Orris root extract	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Oxo-isophorone	1	S				Jing and Xian, 1999
Oxolamine citrate	9				S	Dalhamn, 1969
Oxystarch $\Rightarrow$ dialdehyde starch						
Palladium	9	S S, M 7–9			S	Bryant <i>et al.</i> , 1979 Collins <i>et al.</i> , 1981
Palladium nitrate	9	M 29				Kossack, 1987
Palladium salts	9	S, M 50				Norman and Bryant, 1975
Palmarosa oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Palmitic acid	1	S				Schmeltz <i>et al.</i> , 1978
Parsley oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Peach concentrate	1	S				Bavley and Robb, 1969
Pectin	1, 6		S S S S			Bell <i>et al.</i> , 1966 Gilbert and Lindsey, 1957 Kratchanova <i>et al.</i> , 1995 Schlotzhauer <i>et al.</i> , 1967 Sjöberg and Pyysalo, 1985 Stoilova <i>et al.</i> , 1994
ω -Pentadecalactone	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
2,3-Pentanedione	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Pentyl 2-(1-hydroxycyclohexyl)-acetate $\Rightarrow$		ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate				
Pentyl 3-hydroxy-3-methyl-3-phenylpropionate $\Rightarrow$		ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate				
Peppermint leaves	1		S			Kröller, 1970
Peppermint oil	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Pepper oil, black	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Perfume	1	M 1 M 51				An <i>et al.</i> , 1996 Ogawa, 1998
Perlite	6	M 3				Biggs <i>et al.</i> , 1998
Petitgrain oil	1	M 63		M 63		Carmines, 2002 ^c
Petitgrain oil, terpeneless	1	M 63		M 63		Carmines, 2002 ^c
α -Phellandrene	1		S			Robb <i>et al.</i> , 1964
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Phenethyl acetate	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Phenethyl alcohol	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Phenethyl butyrate	1	M 63		M 63		Carmines, 2002 ^c
Phenethyl isobutyrate	1	M 63		M 63		Carmines, 2002 ^c
Phenethyl isovalerate	1	M 63		M 63		Carmines, 2002 ^c
Phenethyl phenylacetate	1	M 63		M 63		Carmines, 2002 ^c
Phenol	9	S				Bentley and Burgan, 1960
Phenylacetaldehyde	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Phenylacetic acid	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
		M 62, 63		M 62, 63		Carmines, 2002 ^c
2-Phenyl-2-butenal	1	M 63		M 63		Carmines, 2002 ^c
4-Phenyl-3-buten-2-one	1	M 63		M 63		Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Phenyl disulfide	9	S				Burton and Benner, 1972
Phenylmethyl-oxadiazole (PMO)	9	S			S S S	Dalhamn and Rylander, 1971 Jones <i>et al.</i> , 1972 Jones <i>et al.</i> , 1973 Marmor and Minnemeyer, 1975 NCI, Report No. 4, 1980 Rylander, 1971 Rylander, 1973
Phenylpropionic acid	1	S				Burton and Benner, 1972
Phenyl sulfide	9	S				Burton and Benner, 1972
Phenylvinylloxadiazole	9				S	Dalhamn and Rylander, 1971
Phosphoric acid	2	M 1 S				An <i>et al.</i> , 1996 Stedman <i>et al.</i> , 1969
Phytosterols	9	S				Schmeltz <i>et al.</i> , 1978
Pineapple juice	1			M 61		Gaworski <i>et al.</i> , 1998
Pineapple juice concentrate	1			M 60		Gaworski <i>et al.</i> , 1999a
Pinene	1	S				Bavley and Robb, 1969
α-Pinene	1	M 62		M 62		Carmines, 2002 ^c
β-Pinene	1	M 62		M 62		Carmines, 2002 ^c
Pine needle oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Pine oil, scotch	1	M 62		M 62		Carmines, 2002 ^c
δ-Piperitone	1	M 62		M 62		Carmines, 2002 ^c
Piperonal	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Pipsissewa leaf	1			M 61		Gaworski <i>et al.</i> , 1998
Plasticiser	4	M 12 M 18 M 36, 37				Dontenwill <i>et al.</i> , 1972 Dontenwill <i>et al.</i> , 1976 Miano and Keith, 1976
Platinum	9	S				Bryant <i>et al.</i> , 1979
Polyethylene glycol	2		S			Kröller, 1965a
Polyethylene glycols (Carbowax)	9	S				Bilimoria and Nisbet, 1975
Polygalacturonic acid	9		S			Schlotzhauer <i>et al.</i> , 1967
Polypropylene glycol	2	S				Bilimoria and Nisbet, 1975
Potassium acetate	3	S S				Aksu, 1969 Keritsis, 1981
Potassium bromate	9	S				Bentley and Burgan, 1960
Potassium bromide	9	S				Bentley and Burgan, 1960
Potassium carbonate	3, 6	S S S				Burdick <i>et al.</i> , 1969 Burton, 1969 Burton and Benner, 1972
Potassium chlorate	9	S S S				Burdick <i>et al.</i> , 1969 Burton, 1969 Burton and Benner, 1972
Potassium chloride	3, 6	S S				Bentley and Burgan, 1960 Crosthwaite <i>et al.</i> , 1979
Potassium citrate	3, 5	M 1 M 5 M 27 S				An <i>et al.</i> , 1996 Briskin, 1979 Jodl, 1969 Keritsis, 1981
Potassium ethylvanillin-5-carboxylate	⇒	5-carboxyvanillin				
Potassium iodide	9	S				Bentley and Burgan, 1960
Potassium lactate	3	S				Aksu, 1969
Potassium malate	3	S				Aksu, 1969

Table 2 (contd.)

[illegible]

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Rhizome (powder)	6	M 51				Ogawa, 1998
Rhodinol $\Rightarrow$ citronellol						Carmines, 2002 ^c
Rose absolute	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Rose leaves	1		S			Kröller, 1967
Rose oil, bulgarian, true otto	1	M 63		M 63		Carmines, 2002 ^c
Rum	1	M 62, 63		M 62, 63 M 61		Carmines, 2002 ^c Gaworski <i>et al.</i> , 1998
Rum ether	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Rutin	9	S	S			Bell <i>et al.</i> , 1966 Carmella <i>et al.</i> , 1984 Schlotzhauer <i>et al.</i> , 1982
Sage oleoresin	1	M 63		M 63		Carmines, 2002 ^c
Salicylaldehyde	1	M 62, 63		M 61 M 62, 63		Gaworski <i>et al.</i> , 1998 Carmines, 2002 ^c
Sandalwood oil	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Sandalwood oil, yellow	1	M 63		M 63		Carmines, 2002 ^c
Sclareolide	1	M 62		M 62		Carmines, 2002 ^c
Sepiolite	9	M 1				An <i>et al.</i> , 1996
Shellac	6		S			Kröller, 1966d
Silver nitrate	9	S				Bentley and Burgan, 1960
β -Sitosterol	1	S				Cheng, 1973
Sodium acetate	1, 3		S			Kröller, 1966b
Sodium alginate	6	M 3				Biggs <i>et al.</i> , 1998
Sodium antimonate	9	S				Burton and Benner, 1972
Sodium benzoate	5			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Kröller, 1970
Sodium bicarbonate	6	M 5		S		Briskin, 1979
Sodium borate	9	S				Baldry <i>et al.</i> , 1988
Sodium citrate	3, 5	S M 5 M 27				Baldry <i>et al.</i> , 1988 Briskin, 1979 Jodl, 1969 Kröller, 1966b Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Sodium dichromate	9	S				Burton and Benner, 1972
Sodium ethylvanillin-5-carboxylate	$\Rightarrow$	5-carboxyvanillin				
Sodium fluoride	9	S				Burton and Benner, 1972
Sodium glycerophosphate	9		S			Kröller, 1966d
Sodium hydrogen carbonate	9	S				Burton and Benner, 1972
Sodium hydroxide	3, 8	M 39 M 47			M 39 M 47	NCI, Report No.1, 1976 NCI, Report No. 4, 1980
Sodium iodate	9	S				Burton and Benner, 1972
Sodium lactate	1, 3		S			Kröller, 1966b
Sodium malate	3	S				Baldry <i>et al.</i> , 1988
Sodium molybdate	9	S				Burton and Benner, 1972
Sodium nitrate	3	S S S S S, M 14 S, M 17			S S	Adams <i>et al.</i> , 1984 Burton, 1969 Burdick <i>et al.</i> , 1969 Burton and Benner, 1972 Dontenwill <i>et al.</i> , 1972 Dontenwill, 1974 Dontenwill <i>et al.</i> , 1976

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Sodium nitrate (contd.)		S			S	Hoffmann and Wynder, 1967
		S			S	Hoffmann and Wynder, 1968
		S				Johnson <i>et al.</i> , 1973
		S				Klimisch, 1972
		S			S	McCoy and Rosenkranz, 1982
		S				Morie and Sloan, 1973
		S				Sloan and Kiefer, 1969
		S				Terrell and Schmeltz, 1968
		S				Terrell and Schmeltz, 1970
		S			S	Wynder and Hoffmann, 1969
Sodium nitrite	9	S				Bentley and Borgan, 1960
		S				Burdick <i>et al.</i> , 1969
		S				Burton, 1969
		S				Burton and Benner, 1972
Sodium periodate	9	S				Burton and Benner, 1972
Sodium permanganate	9	S				Burton and Benner, 1972
Sodium phosphate hydrate	3, 6, 8	M 26				Eicher and Müller, 1985
Sodium stannate	9	S				Burton and Benner, 1972
Sodium tetraborate	3, 5, 9	S				Bentley and Borgan, 1960
Sodium thiocyanate	9	S				Burton and Benner, 1972
Sodium thiosulfate	9	S				Lakritz <i>et al.</i> , 1972
Sodium vanadate	9	S				Burdick <i>et al.</i> , 1969
		S				Burton, 1969
		S				Burton and Benner, 1972
Sodium vanillin-5-carboxylate	⇒ 5-carboxyvanillin					
Sorbic acid	5	M 15				Dontenwill <i>et al.</i> , 1972
Sorbitol	1, 2	S				Aksu, 1969
		M 4				Billimoria and Nisbet, 1975
		M 6				Carugno <i>et al.</i> , 1971
		S	S			Kröller, 1966d
		S				Pyriki <i>et al.</i> , 1965
						Smit, 1970
Spearmint oil	1			M 61 M 60		Gaworski <i>et al.</i> , 1998
						Gaworski <i>et al.</i> , 1999a
Starch	1, 6	S	S			Bell <i>et al.</i> , 1966
			S			Crosthwaite <i>et al.</i> , 1979
			S			Gilbert and Lindsey, 1957
			S			Kröller, 1966a
Stearic acid	1	M 28 M 51 S				Komatsu, 1997
						Ogawa, 1998
						Schmeltz, 1978
Storax	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Styrax	1, 6			M 61		Gaworski <i>et al.</i> , 1998
Styrax extract	1, 6	M 62, 63		M 62, 63		Carmines, 2002 ^c
Styrax gum	1, 6			M 60		Gaworski <i>et al.</i> , 1999a
Sucrose	1, 2	S	S			Bell <i>et al.</i> , 1966
		S				Gager <i>et al.</i> , 1971a
						Gager <i>et al.</i> , 1971b
			S			Gilbert and Lindsey, 1957
			S			Kröller, 1967
		M 54				Saint-Jalm <i>et al.</i> , 2000
			S			Schlotzhauer <i>et al.</i> , 1982
			S			Schlotzhauer <i>et al.</i> , 1985
			S			Schlotzhauer <i>et al.</i> , 1986
		M 57				Tiggelbeck and Manes, 1976
			S			Tomasik, 1989
		M 62, 63		M 62, 63		Carmines, 2002 ^c
Sucrose ester	1		S			Schlotzhauer <i>et al.</i> , 1986
Sucrose octaacetate	1			M 61 M 60		Gaworski <i>et al.</i> , 1998
						Gaworski <i>et al.</i> , 1999a

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Sugar	1, 2	S M 31–34 S, M 41–44		S S		Jenkins <i>et al.</i> , 1980 McAdam, 1997 NCI, Report No. 3, 1977 Sato <i>et al.</i> , 1979
(Invert sugar)	1, 2	M 62		M 62		Carmines, 2002 ^c
Sugar alcohol	2			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Sugar: corn syrup	1	M 63, 64		M 63, 64		Carmines, 2002 ^c
Sulfite pulp	6	M 40 M 46, 47, 49			M 40 M 46, 47	NCI, Report No. 1, 1976 NCI, Report No. 4, 1980
Sulfuric acid	1, 8	S				Stedman <i>et al.</i> , 1969
Tagetes oil	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Tangerine oil	1	M 63		M 63		Carmines, 2002 ^c
Tartaric acid	1, 3, 5, 6	M 28		M 61 M 60		Komatsu, 1997 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Tartaric acid (disodium salt)	1, 3, 5, 6		S			Kröller, 1966b
α-Terpineol	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Terpinolene	1	M 62		M 62		Carmines, 2002 ^c
Terpinyl acetate	1	M 63		M 63		Carmines, 2002 ^c
Tetracosane	9		S			Bell <i>et al.</i> , 1966
1,5,5,9-Tetramethyl-13-oxatricyclo-(8.3.0.0)-(4,9) tridecane	1			M 60 M 61		Gaworski <i>et al.</i> , 1999a Gaworski <i>et al.</i> , 1998
2,3,5,6-Tetramethylpyrazine	1	M 63		M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Thiabendazole	5	S	S			Kröller, 1968 Kröller, 1969
Thyme oil, white	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Thymol	1	S				Bavley and Robb, 1969
Titanium dioxide	3, 6, 7	M 11 M 26				Dontenwill <i>et al.</i> , 1972 Eicher and Müller, 1985
Titanium oxide	3, 6, 7	M 30				Matsushita and Shinozaki, 1980
Titanyl chloride	9	M 39			M 39	NCI, Report No.1, 1976
Tobacco (highly methylated)	9	M 10				Detert and Ruchholz, 1974
Tobacco extract	1	M 32, 34				McAdam, 1997
Tocopherols	1	M 63		M 63		Carmines, 2002 ^c
<i>o</i> -, <i>m</i> -, <i>p</i> -Tolualdehydes	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
Tolu balsam gum and extract	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Toluene	9	S				Bavley and Robb, 1969
<i>p</i> -Tolyl acetate	1	M 62		M 62		Carmines, 2002 ^c
<i>p</i> -Tolyl isobutyrate	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
<i>p</i> -Tolyl phenylacetate	1	M 63		M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Tonka bean powder	1		S			Higman, H.C. <i>et al.</i> , 1974
Tragacanth	6		S S			Kröller, 1965b Sjöberg and Pyysalo, 1985
Triacetin	4	M 3		M 61 M 60		Biggs <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
			S			Kröller, 1968

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Triacetin (contd.)		S S M 62		M 62		Lyerly, 1967 Mathis, 1983 Carmines, 2002 ^c
Triethyl citrate	8			M 61		Gaworski <i>et al.</i> , 1998
Triethylene glycol	2	M 6	S			Carugno <i>et al.</i> , 1971 Kröller, 1964b
Triethyl orthoformate	9	S				Burton and Benner, 1972
Triglycerol	2		S			Kröller, 1966d
4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-2-en-4-one	1	M 63		M 60 M 63		Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
2,6,6-Trimethylcyclo-hex-2-ene-1,4-dione	1			M 60 M 61		Gaworski <i>et al.</i> , 1999a Gaworski <i>et al.</i> , 1998
4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one	1	M 62, 63		M 62, 63		Carmines, 2002 ^c
2,3,5-Trimethylpyrazine	1			M 61 M 60 M 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Trisodium phosphate	3, 6, 8, 9	S				Stedman <i>et al.</i> , 1969
Trisodium vanadate	9	S				Burton and Benner, 1972
γ-Undecalactone	1	M 38 M 63		M 63		Miranda <i>et al.</i> , 1999 Carmines, 2002 ^c
Urea	1	S M 19–24 S S M 62		M 62		Bentley and Burgan, 1960 Eicher and Müller, 1985 Mariner <i>et al.</i> , 2000 Pintaske, 1981 Carmines, 2002 ^c
Valeraldehyde	1	M 62		M 62		Carmines, 2002 ^c
Valerian root	1			M 61 M 60		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a
Valerian root extract	1	M 63		M 63		Carmines, 2002 ^c
Valerian root oil	1	M 63		M 63		Carmines, 2002 ^c
Valeric acid	1	M 62		M 62		Carmines, 2002 ^c
γ-Valerolactone	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Vanilla extract	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Higman, H.C. <i>et al.</i> , 1974 Carmines, 2002 ^c
Vanilla oleoresin	1	M 63		M 63		Carmines, 2002 ^c
Vanilla roots	1		S			Kröller, 1967
Vanillin	1	S S S M 38 M 62, 63 S S		M 61 M 60 M 62, 63		Bavley and Robb, 1969 Chan <i>et al.</i> , 1992 Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Green <i>et al.</i> , 1989 Kato and Shibayama, 1962 Miranda <i>et al.</i> , 1999 Carmines, 2002 ^c Stotesbury <i>et al.</i> , 1999 Stotesbury <i>et al.</i> , 2000
Veratraldehyde	1			M 61 M 60 M 62, 63		Gaworski <i>et al.</i> , 1998 Gaworski <i>et al.</i> , 1999a Carmines, 2002 ^c
Vetiver oil	1	M 63		M 63		Carmines, 2002 ^c
Walnut hull extract	1	M 62		M 62		Carmines, 2002 ^c
Wetting agent	2	M 36, 37				Miano and Keith, 1976
Wine, Sherry	1	M 62		M 62		Carmines, 2002 ^c

Table 2 (contd.)

Ingredients	Classification Table 1 ^a	MSS Tables 3 & 4 ^b	Pyrolysis Table 5 ^b	Biological activity		Reference(s)
				Table 6 ^b	Table 7 ^b	
Wood pulp	6	M 39			M 39	NCI, Report No.1, 1976
Woodruff	1		S			Kröller, 1967
Yellow wood extract	7		S			Kröller, 1966c
			S			Kröller, 1968
Zeolite Y	9	S				Meier and Siegmann, 1999
Zinc nitrate	9	S				Bentley and Burgan, 1960
Zinc oxide	9	S, M 43–45			S, M 45	NCI, Report No. 3, 1977
		S				Norman <i>et al.</i> , 1973
Zirconium salts	9	M 30				Matsushita and Shinozaki, 1980

^aClassification according to Table 1.

^bTables 2 to 7: S = single substance tested, M xx = substance tested in mixture with other ingredients. Numbering of mixtures, see relevant tables.

^cCarmines, 2002: stands on behalf of the following series of publications: Carmines, 2002; Römer *et al.*, 2002; Rustemeier *et al.*, 2002 and Vanscheeuwijck *et al.*, 2002.

Table 3. Influence of ingredients on the chemical composition of cigarette mainstream smoke (MSS): single substances

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Acetophenone (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	N.d.	Bavley and Robb, 1969 (P)
Alanine	5% (w/w)	Cigarette ("bright yellow" or "Matsukawa" tobacco)	n.r.	n.d.	n.d.	"Bright Yellow" acrylonitrile: — acetone: 15.8 µg/puff (180% ↗) isobutyronitrile: 2.8 µg/puff (260% ↗) propionitrile: 6.5 µg/puff (230% ↗) n-butyronitrile: 1.3 µg/puff (140% ↗) "Matsukawa" acrylonitrile: 1.0 µg/puff (20% ↘) acetone: 26.0 µg/puff (130% ↗) isobutyronitrile: 2.7 µg/puff (100% →) propionitrile: 11.4 µg/puff (140% ↗) n-butyronitrile: 3.0 µg/puff (330% ↗) CO: 11.2% ↗ "tar": 2.5% ↗ nicotine: 3.6% ↗	Kaburaki et al., 1969
Aluminium sulfate	3.5% (w/w)	Cigarette paper	Impregnation with an aqueous solution	n.d.	n.d.	CO: 11.2% ↗ "tar": 2.5% ↗ nicotine: 3.6% ↗	Baldry et al., 1988
γ -Aminobutyric acid	5% (w/w)	Cigarette ("bright yellow" or "Matsukawa" tobacco)	n.r.	n.d.	n.d.	"Bright Yellow" acrylonitrile: + acetone: 15.2 µg/puff (180% ↗) isobutyronitrile: 3.2 µg/puff (290% ↗) propionitrile: 5.8 µg/puff (210% ↗) n-butyronitrile: 1.4 µg/puff (160% ↗) "Matsukawa" acrylonitrile: 0.7 µg/puff (50% ↘) acetone: 22.0 µg/puff (110% ↗) isobutyronitrile: 3.9 µg/puff (140% ↗) propionitrile: 9.9 µg/puff (120% ↗) n-butyronitrile: 3.5 µg/puff (390% ↗)	Kaburaki et al., 1969
Ammonium ceric sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium chromic sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium cobalt sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium compounds	n.r.	Cigarette tobacco	n.r.	Smoke ammonia: 6.1–11.9 µg/cig increase after addition of ammonia compounds.	n.d.	No signif. diff. in smoke pH: 5.3–5.4 nicotine: 0.81 mg/cig (9% ↗)	Ellis et al., 1999 (A)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Ammonium ferric sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium ferrous sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium hexachloropalladate	0.06% (w/w) 0.02–0.12% (w/w) 0.02–0.12% (w/w)	Tobacco blend (cased)	Mixture of tobacco blend with (NH ₄) ₂ PdCl ₆ ⇒ simulation of cigarette pyrolysis	n.d.	n.d.	0.06% : PAH 32% ↘ 0.02–0.12%: PAH 14–40% ↘ (0.1% nitrate content in tobacco) PAH 18–43% ↘ (0.59% nitrate content in tobacco)	Bryant <i>et al.</i> , 1979 (P)
Ammonium hydrogen carbonate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 1% ↗ "tar": 1% ↗ nicotine: 2% ↗ phenol: 16% ↗ o-cresol: 43% ↗ <i>m</i> -, <i>p</i> -cresol: 11% ↗ B[a]P: 38% ↗	Burton and Benner, 1972
Ammonium hydroxide	11 mg/cig	Tobacco	n.r.	n.r.	n.r.	smoke-pH: 7.8 (39.3% ↗)	Stedman <i>et al.</i> , 1969
Ammonium molybdate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium nickel sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium perchlorate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Ammonium phosphate	5%	Reconstituted tobacco sheet	Incorporation during the slurry process. Preparation of cigarettes from treated and non-treated sheets	n.d.	n.d.	Low density sheet (values refer to the tobacco consumed) DPM: 18.4 mg/g (34.3% ↗) nicotine: 1 mg/g (100% ↗) B[a]P: 0.027 µg/g (28.6% ↗) phenol: — (control: 7 µg/g) CO: 27 mg/g (28.6% ↗) NO _x : — (control: 9 µg/g) acrolein: 110 µg/g (266% ↗)	Halter and Ito, 1972
Ammonium phosphate	n.r.	Tobacco	n.r.	n.d.	n.d.	Slight reduction of CO	Grant, 1980 (A)
Ammonium sulfamate	4%	Tobacco	n.r.	n.d.	n.d.	B[a]P: 1.3 µg/100 cig (62.5% ↗)	Pyriki <i>et al.</i> , 1965

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Ammonium sulfamate	4.25%	Cigarette paper	Manufacture of cigarettes with the treated paper	n.d.	n.d.	Reduction of anthracene, B[a]P, fluoranthene and pyrene	Lindsey <i>et al.</i> , 1959
Ammonium sulfamate	5.7%	Cigarette paper	n.r.	n.d.	n.d.	PAH-values (per 100 cigarettes): B[a]P: 2.1 µg (5% ↗) pyrene: 7.5 µg (34.8% ↘) methylpyrene: 10.0 µg (11.1% ↗) anthracene: 10.8 µg (1.9% ↗)	Pyriki <i>et al.</i> , 1965
Ammonium sulfamate	4.25%	Cigarette paper	Impregnation	n.d.	n.d.	No significant reduction of B[a]P formation by ammonium sulfamate	Cuzin <i>et al.</i> , 1960
Ammonium sulfamate	7 mg/cig	Cigarette paper	Incorporation into a commercial cigarette paper. Cigarette smoked to 23 mm butt	n.d.	n.d.	"tar": 26.0 mg/cig (26% ↗) nicotine: 1.10 mg/cig (29% ↗) B[a]P: 1.05 ppm (6% ↘) B[a]A: 1.57 ppm (7% ↘) phenanthrene: 21.2 ppm (1% ↗) chrysene: 1.9 ppm (14% ↘) fluorene: 12.1 ppm (28% ↘) dimethylnitrosamine: 108 ng/cig (8% ↘) methylethylnitrosamine: 42 ng/cig (11% ↘) indole: 12.3 µg/cig (11% ↗) 3-methylindole: 12.2 µg/cig (3% ↗) acetaldehyde: 0.94 mg/cig (6% ↘) acrolein: 0.085 mg/cig (13% ↘) formaldehyde: 0.026 mg/cig (13% ↘) HCN: 0.223 mg/cig (10% ↗) NO _x : 0.425 mg/cig (12% ↗)	Michelson and Rathkamp, 1974
Ammonium sulfamate	15.7%	Cigarette paper	Manufacture of cigarettes with treated and untreated cigarette paper	n.d.	n.d.	B[a]P/100 cigarettes test cigarettes (different storage times) 15 min: 3.85 µg (63.8% ↗) 1 d: 2.95 µg (25.5% ↗) 3 d: 3 µg (27.7% ↗) 1 week: 2.95 µg (25.5% ↗) 2 weeks: 2.75 µg (17% ↗) 4–5 weeks: 2.95 µg (25.5% ↗) 6 weeks: 2.8 µg (19.1% ↗) <i>Phenol/100 cigarettes</i> test cigarettes (storage times not listed) 23.5 mg (113.6% ↗) 18.5 mg (68.2% ↗) 16.8 mg (52.7% ↗) 14.0 mg (27.3% ↗) 12.9 mg (17.3% ↗)	Hoffmann and Wynder, 1968

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Ammonium sulfamate	4.25%	Cigarette paper	Dipping in an aqueous solution			28 and 31 µg B[a]P in "tar" (54–60% ↗) (400 cigarettes were smoked for every single measurement)	Alvord and Cardon, 1956
Ammonium sulfamate	4.25%	Cigarette paper	Impregnation of cigarette paper	n.d.	n.d.	7 µg B[a]P (60% ↗)	Candeli <i>et al.</i> , 1960
Ammonium sulfamate	4% (w/w) 5% (w/w)	Cigarette paper and/or tobacco	Impregnation of the paper and spraying of an aqueous solution on tobacco	n.d.	n.d.	B[a]P in smoke from 500 g of cigarettes (mean value of 3 approaches) test cigarette (tobacco + additive, untreated paper): 1.4 µg (72% ↗) test cigarette (tobacco untreated, paper + additive): 7.9 µg (↔)	Bentley and Burgan, 1960
Ammonium tetrachloropalladate	0.06%, 0.05% (w/w) (calculated as metal)	Tobacco blend (cased)	Mixture of tobacco blend with (NH ₄) ₂ PdCl ₄ ⇒ simulation of cigarette pyrolysis	n.d.	n.d.	0.06%: PAH 22% ↗ (0.1% nitrate content in tobacco) 0.05%: PAH 28% ↗ (0.59% nitrate content in tobacco)	Bryant <i>et al.</i> , 1979 (P)
Ammonium vanadate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 16.5% ↗ "tar": 17.1% ↗ nicotine: 8.8% ↗ phenol: 21.8% ↗ o-cresol: 2.5% ↗ m-, p-cresol: 20.9% ↗ B[a]P: 52.3% ↗	Burton and Benner, 1972
Ammonium vanadate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 56% ↗ phenol: 80% ↗ o-cresol: 90% ↗ m-, p-cresol: 50% ↗ B[a]P: 260% ↗ TPM: 26% ↗	Burdick <i>et al.</i> , 1969
Ammonium vanadate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 56% ↗ phenol: 80% ↗ o-cresol: 90% ↗ m-, p-cresol: 50% ↗ B[a]P: 260% ↗ TPM: 26% ↗	Burton, 1969
Anethole	780 µg/cig	Tobacco	Spraying with an acetone solution	52 and 65 µg/cig ⇒ transfer rate: 6.6 and 8.3%	n.d.	n.d.	Van Auken <i>et al.</i> , 1979 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Anethole released from: poly(1-anisyl-1-propyl allyl carbonate)	780–7800 µg/cig	Tobacco	Spraying with an acetone solution	Anethole delivery into MSS polymer 780 µg/cig ⇒ 5.9 µg/cig polymer 1560 µg/cig ⇒ 11.5 µg/cig polymer 3900 µg/cig ⇒ 23.5 µg/cig polymer 7800 µg/cig ⇒ 60 and 88 µg/cig (2 approaches)	n.d.	n.d.	Van Aken et al., 1979 (P)
Anethole (5.2% in α-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Anethole (in tri-o-thymoid)	1%	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Anethole	3.3 mg	Cigarette filter	Manufacture of a cellulose acetate filter rod comprising 10 mg anethole resin/cm	fresh: 0.46 mg/cig transfer of anethole flavour: 13.9% aged: 0.38 mg/cig transfer of anethole: 11.5%	n.d.	fresh: TPM: 32 mg aged (7 d): TPM: 33 mg	Badgett and Osmalov, 1971 (P)
Anethole-maleic anhydride (31.6%)	0.75 g	Tobacco (100 g)	Spraying	n.d.	anethole: 0.12 mg/cig transfer rate: 5.1%	n.d.	Robb et al., 1964
Aniline	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Anisaldehyde	85 µCi/cig (65 µg/cig)	Cigarette	Manual syringe injection of cigarettes with ¹⁴ C-anisaldehyde (186 mCi/mmol)	TPM: 11.6% vapour phase: 0.1%	Extent of decomposition: 8.6%	n.d.	Green et al., 1989
p-Anisaldehyde	5000 µg/cig (labelled or unlabelled) or 1 mg (capillary tube)	Cigarette + capillary tube	Injection of an ethanolic solution (25 µL) into the cigarette with labelled ¹³ C and ¹⁸ O p-anisaldehyde	Degradation of p-anisaldehyde at different temperatures 200 °C: 97.1% ⇒ pyrolysis cond. 200–400 °C: 97% ⇒ pyrolysis cond. 200–800 °C: 69.1% ⇒ pyrolysis cond. smoke [¹³ C]: 99.1% Total extent of transfer to the mainstream TPM (intact additive and degradation products): 8.1%	Further combustion products: anisole [¹³ C]: 0.3% 200–800 °C: 7.6% phenol [¹³ C]: 0.6% 200–800 °C: 5.9% benzaldehyde 200–800 °C: 3.7% methyl-4-hydroxybenzoate 200 °C: 1.2% 200–400 °C: 1% 200–800 °C: 0.9%	n.d.	Stotesbury et al., 2000

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
<i>p</i> -Anisaldehyde (5000 µg/cig) (contd.)					methyl-4-methoxybenzoate 200 °C: 0.5% 200–400 °C: 0.9% 200–800 °C: 1.2% 4-hydroxy-benzaldehyde 200–800 °C: 1.2%		
<i>p</i> -Anisaldehyde	1 mg	Capillary tube (modelling cigarette combustion)	No application to tobacco	Predicted transfer of <i>p</i> -anisaldehyde: 97% (400 °C)	<i>Further combustion products:</i> methyl <i>p</i> -hydroxybenzoate: 1% methyl-4-methoxybenzoate: 0.9% 4-methoxyphenol: 0.3% anisic acid: 0.3% 1,1-dimethoxy-2-propanal: 0.2% 1,1-dimethoxy-2-phenylpropane: 0.1% 2-methoxyphenol: 0.1%	n.d.	Statesbury <i>et al.</i> , 1999
Anisole	1 mg	Capillary tube (modelling cigarette combustion)	No application to tobacco	Predicted transfer of anisole: 97% (200 °C, 2% and 10% O ₂)	<i>Further combustion products:</i> o-methylanisole: 1.6% <i>p</i> -methylanisole: 1.5% Extent of decomposition: 0%	n.d.	Statesbury <i>et al.</i> , 1999
Anisole	8.7 µCi/cig (8.7 µg)	Cigarette	Manual syringe injection of cigarettes with ¹⁴ C-labelled anisole (112 mCi/mmol)	TPM: 3.9% vapour phase: 9.3%		n.d.	Green <i>et al.</i> , 1989
Anthracene	790 × 10 ³ cpm/cig	Cigarette	Hypodermic syringe injection of 80 µL of anthracene-9- ¹⁴ C containing solutions	n.d.	Activity recovered particulate: 20.1% vapour: 0.2% butt: 39.2%	n.d.	Thornton and Valentine, 1968
Ascorbic acid	0–5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Aspartic acid	5% (w/w)	Cigarette ("bright yellow" or "Matsukawa" tobacco)	n.r.	n.d.	n.d.	"Bright Yellow" acrylonitrile: — acetonitrile: 13.4 µg/puff (160% ↗) isobutyronitrile: 3.4 µg/puff (130% ↗) propionitrile: 5.0 µg/puff (180% ↗) <i>n</i> -butyronitrile: 1.4 µg/puff (160% ↗)	Kaburaki <i>et al.</i> , 1969

Table 3 (contd.)

Ingredient	Experimental design		Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Aspartic acid (5%, contd.)					"Matsukawa" acrylonitrile: 0.7 µg/puff (50% ↗) acetonitrile: 21.1 µg/puff (110% ↗) isobutyronitrile: 3.4 µg/puff (130% ↗) propionitrile: 8.1 µg/puff (100% →) n-butyronitrile: 3.4 µg/puff (380% ↗)
Azo-bis-isobutyronitrile	5%	Tobacco	Spraying of an aqueous solution	n.d.	TPM: 7.2% ↗ "tar": 9.8% ↗ nicotine: 32.1% ↗ phenol: 14.1% ↗ o-cresol: 36% ↗ m-, p-cresol: 24.7% ↗ B[a]P: 69.2% ↗
Azo-bis-isobutyronitrile (Vazo)	10%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	<i>Fifth puff</i> (35 mL) H₂: 0.68 mol% (17.1% ↗) O₂: 15.08 mol% (7.6% ↗) CO: 1.42 mol% (20.2% ↗) CO₂: 4.64 mol% (15% ↗) NO + NO₂: 12.1 µg (20.9% ↗) N₂O: < 1 µg (→) HCN: 22.3 µg (68.9% ↗) H₂S: 2.7 µg (80% ↗) SO₂: 3.3 µg (73.7% ↗) CH₄: 59.9 µg (14.3% ↗) C₂H₆: 21.4 µg (5.8% ↗) ethylene: 8.7 µg (18.7% ↗) acetaldehyde: 30.2 µg (35.6% ↗) acetone: 35.2 µg (30.4% ↗) acetonitrile: 9.1 µg (28.9% ↗) acrolein: 4.5 µg (21.1% ↗) formaldehyde: 3.4 µg (69.4% ↗) methanol + methyl chloride + methyl acetylene: 13.5 µg (44% ↗)
Barium acetate	5%	Tobacco	Spraying of an aqueous solution	n.d.	TPM: 6.8% ↗ "tar": 7.7% ↗ nicotine: 10.7% ↗ phenol: 11.3% ↗ o-cresol: 128% ↗ m-, p-cresol: 43.8% ↗ B[a]P: 59% ↗

Burton and Benner, 1972

Terrell and Schmeltz, 1970

Burton and Benner, 1972

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Benzaldehyde	52 µCi/cig (104 µg)	Cigarette	Manual syringe injection of cigarettes with ¹⁴ C-labelled benzaldehyde (54 mCi/mmol)	TPM: 8.6% vapour phase: 1.1%	Extent of decomposition: 0%	n.d.	Green <i>et al.</i> , 1989
Benzaldehyde	100–500 µg	Cigarette	Injection of an ethanolic solution 10–50 µL	Predicted transfer of benzaldehyde: 73.5% (200 °C, 2% and 10% O ₂)	<i>Further combustion products:</i> benzoic acid: 26.3% diphenyl ethanedione: 0.1% toluene: 0.05%	n.d.	Statesbury <i>et al.</i> , 1999
Benzoquinone	100 mg/cig	Cigarette	Syringe injection	n.d.	n.d.	TPM: 29.1 mg/cig (27.1% ↗) B[a]P: 0.071 µg/cig (6% ↗) nicotine: 1.54 mg/cig (21.8% ↗) phenol: 266 µg/cig (20.9% ↗)	Lakritz <i>et al.</i> , 1972
Benzothiazyl disulfide	8%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.	<i>Fifth puff (35 mL)</i> H ₂ : 0.08 mol% (90.2% ↗) O ₂ : 17.14 mol% (22.3% ↗) CO: 0.34 mol% (80.9% ↗) CO ₂ : 1.96 mol% (64.1% ↗) NO + NO ₂ : 4.4 µg (71.1% ↗) N ₂ O: < 1 µg (↗) HCN: 4.7 µg (64.4% ↗) H ₂ S: 3.5 µg (133% ↗) SO ₂ : 2.8 µg (47.4% ↗) CH ₄ : 7.5 µg (91.3% ↗) C ₂ H ₆ : 3.3 µg (85.6% ↗) ethylene: 1.7 µg (84.1% ↗) acetaldehyde: 3.9 µg (91.7% ↗) acetone: 3.3 µg (87.8% ↗) acetonitrile: 1.7 µg (86.7% ↗) acrolein: 0.5 µg (91.2% ↗) formaldehyde: 3.4 µg (30.6% ↗) methanol + methyl chloride + methyl acetylene: 1.4 µg (94.2% ↗)	Terrell and Schmeltz, 1970
Benzo[a]pyrene	740 × 10 ³ cpm/cig 418 × 10 ³ cpm/cig	Cigarette	Hypodermic syringe injection of 80 µL of B[a]P-7:10- ¹⁴ C containing solutions	n.d.	740 × 10 ³ cpm/cig particulate: 26.1% vapour: 0% butt: 2.9% 418 × 10 ³ cpm/cig particulate: 22.9% vapour: 0% butt: 2.3%	n.d.	Thornton and Valentine, 1968

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to tobacco	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Bismuth oxide	5.2%	Flue-cured tobacco	Dusting of flue-cured blends (control untreated)	n.d.	n.d.	$\mu\text{g}/100$ cigarettes fluorene: 39 (53% ↗) methylfluorenes: 68 (51.8% ↗) phenanthrene: 35 (51.4% ↗) anthracene: 12 (47.8% ↗) alkyl phenanthrene: 39 (40% ↗) dimethyl phenanthrene: 44 (30.2% ↗) fluoranthene: 11 (35.2% ↗) alkylfluoranthene: 14 (57.6% ↗) pyrene: 7 (41.7% ↗) benzofluorene: 4 (55.6% ↗) alkylbenzofluorene: 9 (47% ↗) B[a]A: 2 (50% ↗) chrysene: 3 (50% ↗) benzofluoranthene: 2 (50% ↗) B[e]P: 1 (↔) B[a]P: 2 (33.3% ↗) TPM: 35 (↔)	Chakraborty <i>et al.</i> , 1971
Borate	10% (w/w)	Tobacco	Spraying of a mixture of boric acid and sodium tetraborate decahydrate (3:7)	n.d.	n.d.	TPM: 30.41 mg/cig (17.5% ↗) nicotine: 1.38 mg/cig (43.9% ↗) phenol: 263 $\mu\text{g}/\text{cig}$ (92% ↗) o-cresol: 35.2 $\mu\text{g}/\text{cig}$ (43.1% ↗) m, p-cresol: 113 $\mu\text{g}/\text{cig}$ (60.7% ↗) B[a]P: 120 ng/cig (91% ↗)	Benner <i>et al.</i> , 1969a
Borate	10%	Tobacco	Spraying of an aqueous solution of boric acid and sodium tetraborate decahydrate (3:7)	n.d.	n.d.	nicotine: 27% ↗ phenol: 150% ↗ o-cresol: 90% ↗ m-, p-cresol: 130% ↗ B[a]P: 100% ↗ TPM: 2% ↗	Burdick <i>et al.</i> , 1969
Borate	10%	Tobacco	Spraying of an aqueous solution of boric acid and sodium tetraborate decahydrate (3:7)	n.d.	n.d.	nicotine: 27% ↗ phenol: 150% ↗ o-cresol: 90% ↗ m-, p-cresol: 130% ↗ B[a]P: 100% ↗ TPM: 2% ↗	Burton, 1969
Borate	10% (w/w)	Cellulose and lignin from tobacco	Spraying of a mixture of boric acid and sodium tetraborate decahydrate (3:7)	n.d.	n.d.	Borate salts are partially responsible for the increased levels of phenol during pyrolysis of borate-treated tobacco	Benner <i>et al.</i> , 1969b

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Boric acid	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 9.4% ↗ "tar": 12.6% ↗ nicotine: 35.3% ↗ phenol: 251% ↗ o-cresol: 215% ↗ m-, p-cresol: 281.8% ↗ B[a]P: 44.9% ↗	Burton and Benner, 1972
1,3-Butylene glycol	3%	Tobacco	Addition to dried tobacco	n.d.	n.d.	nicotine: 2.13–2.96 mg/cig (6–12% ↗) TPM: 43.5 mg/cig (3.5% ↗) dry condensate: 40.4 mg/cig (3.8% ↗)	Smit, 1970
1,3-Butylene glycol (43.5 mg/cig)	3.4%	Cigarette	Addition during casing of cigarette tobacco	n.d.	n.d.	TPM: 60.9 mg/cig (3.6% ↗) polyol: 7.82 mg/cig (6.1% ↗) nicotine: 5.33 mg/cig (10.6% ↗) volatile acids: 2.1 mg/cig (27.1% ↗)	Kobashi <i>et al.</i> , 1965
2,3-Butylene glycol (43.5 mg/cig)	3.4%	Cigarette	Addition during casing of cigarette tobacco	n.d.	n.d.	TPM: 61.8 mg/cig (5.1% ↗) polyol: 6.32 mg/cig (24.1% ↗) nicotine: 5.41 mg/cig (9.2% ↗) volatile acids: 2.08 mg/cig (27.8% ↗)	Kobashi <i>et al.</i> , 1965
2,6-di- <i>tert</i> -Butyl- <i>v</i> -methylphenol	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 36% ↗ "tar": 40% ↗ nicotine: 45% ↗ phenol: 44% ↗ o-cresol: 68% ↗ m-, p-cresol: 55% ↗ B[a]P: 5% ↗	Burton and Benner, 1972
Calcium nitrate	N added as nitrate: 1.8%	Tobacco	Spraying of an aqueous solution with labelled ¹⁵ N calcium nitrate	n.r.	dimethylpyrazine: 15% n.d. pyridine: 13% HCN: 39% acetonitrile: 45% acrylonitrile: 39%		Johnson <i>et al.</i> , 1973
Calcium nitrate	0.27 and 0.64% (w/w) in tobacco	Tobacco blends	Flue-cured or burley tobaccos are sprayed with an aqueous solution	n.d.	0.27%: NO _x : 0.280 mg/cig (900% ↗) 0.64%: NO _x : 0.658 mg/cig (2250% ↗) n.d.	0.27%: catechol: 164 µg/cig (28.1% ↗) 0.64%: catechol: 117 µg/cig (48.7% ↗)	Kallianos <i>et al.</i> , 1968
Calcium oxalate	7.1%	Flue-cured tobacco	Dusting of flue-cured blends (control untreated)	n.d.	n.d.	µg/100 cigarettes fluorene: 47 (43.4% ↗) methylfluorenes: 77 (45.4% ↗) phenanthrene: 48 (33.3% ↗) anthracene: 16 (30.4% ↗) alkyl phenanthrene: 39 (40% ↗)	Chakraborty <i>et al.</i> , 1971

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)	
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products		
Calcium oxalate (7.1%, contd.)					dimethyl phenanthrene: 37 (41.3% ↗) fluoranthene: 14 (17.6% ↗) alkylfluoranthene: 20 (39.4% ↗) pyrene: 9 (25% ↗) benzofluorene: 5 (44.4% ↗) alkylbenzofluorene: 10 (41.2% ↗) B[a]A: 4 (↔) chrysene: 5 (16.7% ↗) benzofluoranthene: 3 (25% ↗) B[a]P: 1 (↔) B[a]P: 2 (33.3% ↗) TPM: 31.5 (10% ↗)		
Carboxymethyl-cellulose	33%	Tobacco	Manufacture of a composition containing tobacco and the additive (dry mixture, 67:33)	n.d.	n.d.	dry "tar": 17.6 mg/cig (29% ↗) acetaldehyde: 34.2 µg/puff (28.4% ↗) acetonitrile: 6.9 µg/puff (58.4% ↗) acrolein: 2.7 µg/puff (53.4% ↗) furan: 1.5 µg/puff (51.6% ↗) propionaldehyde: 3.1 µg/puff (24.4% ↗) acetone: 21.4 µg/puff (24.1% ↗) propionitrile: 1.3 µg/puff (51.9% ↗) isobutyraldehyde: 1.2 µg/puff (45.4% ↗) benzene: 4.1 µg/puff (42.2% ↗)	Miano and Keith, 1976 (P)
Casein hydrolysate	0–8%	Powder (0.1 g) of extracted cigarette tobacco	Mixture with leaf powder or powder from extracted cigarettes	n.r.	n.d.	Slight increase of alkylating activity by casein hydrolysate when pyrolysed in air at 550 °C. No effect when pyrolysed in nitrogen at 750 °C	Crosthwaite et al., 1979
Catalyst (aluminium oxide + molybdenum trioxide)	10%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.	<i>Fifth puff (35 mL)</i> H ₂ : 1.05 mol% (28% ↗) O ₂ : 16.26 mol% (16.1% ↗) CO: 2.49 mol% (39.9% ↗) CO ₂ : 5.74 mol% (5.1% ↗) NO + NO ₂ : 22 µg (44.7% ↗) N ₂ O: < 1 µg (↔) HCN: 12.8 µg (3.1% ↗) H ₂ S: 3.1 µg (106% ↗) SO ₂ : 2.4 µg (26.3% ↗) CH ₄ : 90 µg (28.8% ↗) C ₂ H ₆ : 26.6 µg (16.2% ↗) ethylene: 14.3 µg (33.6% ↗) acetaldehyde: 51 µg (8.7% ↗) acetone: 23.4 µg (13.4% ↗) acetonitrile: 11.4 µg (10.9% ↗) acrolein: 8.2 µg (43.9% ↗) formaldehyde: 5.5 µg (12.2% ↗) methanol + methyl chloride + methyl acetylene: 22.5 µg (6.6% ↗)	Terrell and Schmeltz, 1970

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Cellulose	34.87% carbon content (paper)	Cigarette paper	Preparation of cigarette paper from ¹⁴ C-cellulose	n.d.	Carbon ⇒ MSS gas phase: 20.4% TPM: 9.7%	n.d.	Jenkins <i>et al.</i> , 1980
Cellulose	17–44%	Tobacco blend	Filter paper or powder	n.d.	Increasing gas-phase components with increasing cellulose content: furfuryl, furan, 2-methylfuran, furfural, alcohol, dimethylfuran, acetaldehyde, acrolein, 5-methylfurfural, 3-buten-2-one, methyl acetate, pentadiene, propionaldehyde, isobutyraldehyde, crotonaldehyde, 2-butanone, benzene, butene, propenes, propyne, acetylene, butadiene, acetone, acetonitrile	TPM yield (per g of filler) Added as a homogenate of cellulose powder and leaf tobacco 17% cellulose: 26 mg (8.3% ↗) 44% cellulose: 25 mg (4.2% ↗) Added as filter paper shreds with tobacco homogenate 17% cellulose: 39 mg (62.5% ↗) 28% cellulose: 40 mg (66.6% ↗) 44% cellulose: 44 mg (83.3% ↗) Added as filter paper soaked in tobacco solubles with tobacco homogenate 17% cellulose: 30 mg (25% ↗) 28% cellulose: 31 mg (29.2% ↗) 44% cellulose: 33 mg (37.5% ↗)	Wakeham and Silberman, 1966
Cellulose	3.7 × 10 ⁷ dpm of ¹⁴ C-cellulose	Cigarette	3 g tobacco mixed with 125 mg ¹⁴ C-cellulose from tobacco (10 µCi/mg) ⇒ preparation of cigarettes	n.d.	Conversion of ¹⁴ C-cellulose in tobacco to ¹⁴ C-catechol in MSS: 0.02%; estimated minimum contribution of cellulose to MSS catechol: 7–12%	n.d.	Carmella <i>et al.</i> , 1984
Cellulose	10%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of cigarettes (SEB IV made from reconstituted tobacco sheet: „Schweitzer“ paper process) + cellulose fibers	n.d.	n.d.	Concentration/cigarette TPM: 21.2 mg/cig (15.5% ↗) “tar”: 16.9 mg/cig (14.6% ↗) water: 3.31 mg/cig (21.2% ↗) nicotine: 0.98 mg/cig (16.9% ↗) phenol: 51 µg/cig (22.7% ↗) acetaldehyde: 0.67 mg/cig (21.2% ↗) acrolein: 100 µg/cig (17.4% ↗) isoprene: 274 µg/cig (1.9% ↗) HCN: 225 µg/cig (9.6% ↗) formaldehyde: 44 µg/cig (37.5% ↗) NO _x : 226 µg/cig (4.1% ↗) CO: 15 mL/cig (13.3% ↗) CO ₂ : 21.5 mL/cig (17.9% ↗)	NCI, Report No. 4, 1980

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Cellulose (10%, contd.)						Concentration/g dry condensate indole: 143 mg/g (1.4% ↗) skatole: 277 mg/g (1.1% ↗) B[a]A: 0.85 µg/g (18.1% ↗) B[a]P: 0.61 µg/g (5.2% ↗) o-cresol: 0.82 mg/g (51.9% ↗) m-, p-cresol: 1.82 mg/g (24.7% ↗) colorim. phenols: 5.67 mg/g (4.4% ↗) tot. w-acids: 2.91 meq/g (4.6% ↗) fatty acids: 13.35 mg/g (24.0% ↗) OLL-acids: 8.09 mg/g (39.7% ↗) palmitic acid: 3.94 mg/g (23.1% ↗) stearic acid: 2.5 mg/g (41.2% ↗) neophytadiene: 5.64 mg/g (20.5% ↗) glycerol: 132 mg/g (14.8% ↗) catechol: 5.16 mg/g (3.4% ↗)
Chlorogenic acid	0, 7, 14 and 21 mg/cig	Tobacco	Spraying with 3.4 mL MeOH containing varying amounts of chlorogenic acid ⇒ preparation of cigarettes	n.d.	Estimated minimum contribution of chlorogenic acid to MSS catechol: 13%	n.d.
Chlorophyllin	0–8%	Powder (0.1 g) of extracted cigarette tobacco	Mixture with leaf powder or powder from extracted cigarettes	n.r.	n.d.	Slight increase of alkylating activity by chlorophyllin when pyrolysed in air
Cholesterol	n.r.	Cigarette	Syringe injection of a chloroform solution of cholesterol-4- ¹⁴ C into 62 mm length of a cigarette	Average transfer of ¹⁴ C-labelled cholesterol: 20.27% smoke condensate: 16.25% butt: 4.02% ash: 0.004%	n.d.	n.d.
Cineol (in β- cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.

Carmella et al.,
1984Crosthwaite et
al., 1979

Cheng, 1973

Bavley and
Robb, 1969 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Cinnamyl isovalerate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of cinnamyl isovalerate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 31 (0) 0.89 (0) 0.67 (0) 26 (1) 0.76 (1) 0.42 (1) 23 (2) 0.76 (2) 0.44 (2) 16 (4) 0.66 (4) 0.52 (4) 16 (6) 0.92 (6) 0.71 (6) 18 (8) 0.51 (8) 0.31 (8)	n.d.	n.d.	Mathis, 1983
Cinnamyl propionate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of cinnamyl propionate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 27 (0) 0.82 (0) 0.63 (0) 15 (1) 1.20 (1) 0.46 (1) 12 (2) 0.88 (2) 0.62 (2) 9.5 (4) 0.71 (4) 0.55 (4) 9.6 (6) 0.97 (6) 0.81 (6) 9.9 (8) 0.71 (8) 0.47 (8)	n.d.	n.d.	Mathis, 1983
Citric acid	120 mg/cig	Tobacco	n.r.	n.r.	n.r.	smoke-pH: 5.0 (15.2% ↗)	Siedman et al., 1969
Citronellal (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Citron oil (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Cocoa	1.0% (w/w)	Tobacco blend (flue-cured, burley, Maryland, Turkish, Reconstituted sheet)	Added during casing (powdered form) ⇒ manufacture of cigarettes (SEB III)	n.d.	n.d.	Concentration/cigarette TPM: 29.21 mg/cig (8% ↗) "tar": 25.46 mg/cig (6.1% ↗) water: 1.97 mg/cig (26.8% ↗) nicotine: 1.78 mg/cig (1.1% ↗) phenol: 204.75 μ g/cig (24.8% ↗) acetaldehyde: 1.07 mg/cig (9% ↗) acrolein: 97 μ g/cig (10.2% ↗) isoprene: 505.62 μ g/cig (9.9% ↗) HCN: 305.88 μ g/cig (9.5% ↗) formaldehyde: 32.47 μ g/cig (4.5% ↗) NO _x : 424.4 μ g/cig (2.7% ↗) CO: 15.15 mL/cig (5.9% ↗) CO ₂ : 30.12 mL/cig (24.8% ↗)	NCI, Report No. 3, 1977

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Cocoa (1%, contd.)						Concentration/g dry condensate indole: 845.2 µg/g (82.5% ↗) skatole: 321.8 µg/g (2.2% ↗) BlajA: 1.40 µg/g (0.7% ↗) BlajP: 1.06 µg/g (3.9% ↗) o-cresol: 0.75 mg/g (7.1% ↗) m-, p-cresol: 2.02 mg/g (4.7% ↗) tot. w-acids: 2.31 meq/g (3.1% ↗) fatty acids: 23.50 mg/g (8.7% ↗) OLL-acids: 13.92mg/g (7.7% ↗) palmitic acid: 7.26 mg/g (10.0% ↗) stearic acid: 2.33 mg/g (11.5% ↗) catechol: 6.59 mg/g (27.2% ↗)	
Copper nitrate	1–5% (w/w)	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	BlajP (µg/smoke of 500 g tobacco) 1%: 2.2 µg (64% ↗) 2.5%: 1.3 µg (79% ↗) 5%: 1.45 µg (79.6% ↗, mean value of two measurements)	Bentley and Burgan, 1960
Copper nitrate	5%	Tobacco	Manufacture of treated and untreated cigarettes	n.d.	n.d.	"tar": 26.5 mg/cig (8.3% ↗) BlajP: 1.75 µg/100 cig (54.5% ↗) phenol: 65 µg/100 cig. (33.7% ↗)	Wynder and Hoffmann, 1963
Copper nitrate	5%	Tobacco	Manufacture of treated and untreated cigarettes	n.d.	n.d.	BlajP: 20 µg/cig (31% ↗) phenol: 86 µg/cig (10.4% ↗)	Wynder and Hoffmann, 1969
Copper sulfate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in BlajP content of smoke	Bentley and Burgan, 1960
o-, m-, p-Cresol (in α-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
o-, m-, p-Cresol (in tri-o-thymoid)	1%	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Coumarin (in α-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Coumarin (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Cyclohexanone (in α-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Cyclohexanone (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
p-Cymol (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
p-Cymol (in tri-o-thymoid)	1%	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969(P)
β-Damascenone	n.r.	Cigarette	n.r.	Flavour constituents in smoke decreased to different extents when ventilation was increased	n.r.	Reduction of CO and "tar" deliveries with increasing ventilation	Jing and Xian, 1999 (A)
β-Damascone	n.r.	Cigarette	n.r.	Flavour constituents in smoke decreased to different extents when ventilation was increased	n.r.	Reduction of CO and "tar" deliveries with increasing ventilation	Jing and Xian, 1999 (A)
Diammonium palladium nitrite	0.06%, 0.1% (w/w) (calculated as metal)	Tobacco blend (cased)	Mixture of tobacco blend with (NH ₄) ₂ PdCl ₄ ⇒ simulation of cigarette pyrolysis	n.d.	n.d.	0.06%: PAH 29% ↗ 0.1%: PAH 45% ↗	Bryant <i>et al.</i> , 1979 (P)
Diammonium phosphate (DAP)	0.5%	Cigarette blend	n.r.	n.d.	n.d.	28 µg/cig NH ₃ (75% ↗) smoke pH: 5.5 (1.8% ↗)	Mariner <i>et al.</i> , 2000 (A)
Diammonium platininitrite	0.06% 0.1% (w/w) (calculated as metal)	Tobacco blend (cased)	Mixture of tobacco blend with (NH ₄) ₂ PdCl ₄ ⇒ simulation of cigarette pyrolysis	n.d.	n.d.	0.06%: PAH 6% ↗ 0.1%: PAH 6% ↗	Bryant <i>et al.</i> , 1979 (P)
Diethylamine	140 mg/cig	Tobacco	n.r.	n.r.	n.r.	smoke-pH: 8.1 (44.6% ↗)	Stedman <i>et al.</i> , 1969
Diethylene glycol	2 and 3%	Tobacco	Diluted with water by spraying	n.d.	n.d.	2%: nicotine: 1.19 mg/cig (↔) "tar": 27.1 mg/cig (7.5% ↗) CO: 15.7 mg/cig (5.4% ↗) 3%: nicotine: 1.22 mg/cig (2.5% ↗) "tar": 27.6 mg/cig (9.5% ↗) CO: 16 mg/cig (7.4% ↗)	Stoilova <i>et al.</i> , 1994
Diethylene glycol	6%	Tobacco blend	Sprayed on the tobacco	n.d.	n.d.	Flavoured cigarette blend diethylene glycol - water (1:1): nicotine: 1.43 mg/cig (2.1% ↗) "tar": 27.9 mg/cig (7.3% ↗) CO: 20.8 mg/cig (4% ↗) Unflavoured cigarette blend diethylene glycol - water (1:1): nicotine: 1.2 mg/cig (0.8% ↗) "tar": 27.4 mg/cig (1.8% ↗) CO: 20 mg/cig (11.1% ↗)	Kratchanova <i>et al.</i> , 1995

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on ^{MSS}	
Diethylene glycol	n.r.	Tobacco	Treatment with 2% of aqueous sol	n.d.	n.d.	"tar": 30.7 mg/cig (12.5% ↗)	Aksu, 1969
Dipropylamine	100 mg/cig	Cigarette	Syringe injection in cigarettes with CA-filters and cigarettes with CH-filters	n.d.	n.d.	<i>Non-filter cigarettes</i> TPM: 34.6 mg/cig (41.2% ↗) formic acid: 416 µg/cig (259% ↗) acetic acid: 1229 µg/cig (198% ↗) phenols: 159 µg/cig (15% ↘) <i>Cigarettes + CH-filter</i> TPM: 24.6 mg/cig (43.9% ↗) formic acid: 204 µg/cig (180% ↗) acetic acid: 679 µg/cig (203% ↗) phenols: 122 µg/cig (84.9% ↗) <i>Cigarettes + CA-filter</i> TPM: 21.5 mg/cig (34.4% ↗) formic acid: 142 µg/cig (173% ↗) acetic acid: 536 µg/cig (134% ↗) phenols: 126 µg/cig (27.3% ↗)	Lakritz et al., 1969
Dipropylamine	100 mg/cig	Cigarette	Injection	n.d.	n.d.	<i>Non-filter cigarettes</i> TPM: 30.8 mg/cig (27.3% ↗) pyridine: 26.5 µg/cig (3.6% ↘) nicotine: 2.01 mg/cig (16.2% ↗) smoke pH: 8.2 (46.4% ↗) <i>Cigarettes + CH-filter</i> TPM: 24.7 mg/cig (61.4% ↗) pyridine: 10 µg/cig (108.3 ↗) nicotine: 1.27 mg/cig (13.4% ↗) smoke pH: 7.9 (29.5% ↗) <i>Cigarettes + CA-filter</i> TPM: 24.5 mg/cig (40% ↗) pyridine: 26.2 µg/cig (41.6% ↗) nicotine: 1.11 mg/cig (5.1% ↗) smoke pH: 7.9 (36.8% ↗)	Stedman et al., 1969
Disodium carbonate	40 mg/cig	Tobacco	n.r.	n.r.	n.r.	smoke-pH: 6.4 (14.3% ↗)	Stedman et al., 1969
Disodium hydrogen phosphate	1.2% (w/w)	Cigarette paper	Impregnation with an aqueous solution	n.d.	n.d.	CO: 16.9% ↗ "tar": 3.8% ↘ nicotine: 7.1% ↘	Baldry et al., 1988
Dolomitic limestone	33%	Tobacco	Manufacture of a composition containing tobacco and the additive (dry mixture, 67:33)	n.d.	n.d.	dry "tar": 16.8 mg/cig (32.3% ↘) acetaldehyde: 53.4 µg/puff (11.7% ↗) acetonitrile: 18.5 µg/puff (11.4% ↗) acrolein: 7.5 µg/puff (29.3% ↗) furan: 3.4 µg/puff (9.7% ↗) propionaldehyde: 4.8 µg/puff (17.1% ↗)	Miano and Keith, 1976 (P)

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)																						
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products																							
Dolomitic limestone (33%, contd.)																												
Dotriacontane	0.4 mCi dotriacontane-16,17- ¹⁴ C on tobacco ⇒ 10.8 µCi/cig	Tobacco	Blended tobacco were sprayed with labelled dotriacontane (3.91 mCi/mM) in 25 mL hexane ⇒ preparation of cigarettes	95% of activity in MSS can be attributed to unchanged dotriacontane	Distribution of activity in n.r. MSS (% total activity) CO-CO ₂ : 16.8 nCi ⇒ 0.7% C ₁ -C ₁₀ : 100.8 nCi ⇒ 4.2% C ₁₁ -C ₃₀ : 0 nCi ⇒ 0% C ₃₁ -C ₃₃ : 2300 nCi ⇒ 95.1% >C ₃₃ : 0 nCi ⇒ 0% gas phase: 1.14 µCi ⇒ 10% TPM: 2.09 µCi ⇒ 20% butt: 3.25 µCi ⇒ 30%	acetone: 28.9 µg/puff (2.5% ↗) propionitrile: 2.9 µg/puff (7.4% ↗) isobutyraldehyde: 3.6 µg/puff (63.6% ↗) benzene: 7.5 µg/puff (5.6% ↗)																						
						Jenkins <i>et al.</i> , 1970a																						
Dotriacontane	0.75 mCi dotriacontane-16,17- ¹⁴ C on tobacco	Tobacco filler (cased, blended)	Blended tobacco were sprayed with labelled dotriacontane (3.91 mCi/mM) in 15 mL hexane ⇒ preparation of cigarettes	n.d.	Max. radioactivity in B[a]P: MSS: 4.7 × 10 ⁻¹² Ci (16% ↘) Max. conversion of dotriacontane to B[a]P: MSS: 2.6 × 10 ⁻⁷ (4% ↗) ⇒ Contribution of naturally occurring dotriacontane to B[a]P-formation: 1/1500	n.d.																						
						Jenkins <i>et al.</i> , 1973																						
4-Ethoxy-acetophenone	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of 4-ethoxyacetophenone after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery	n.d.	n.d.																						
				<table><tr><th>Delivery (%)</th><th>25%Dilution</th><th>50% Dilution</th></tr><tr><td>23 (0)</td><td>0.91 (0)</td><td>0.64 (0)</td></tr><tr><td>11 (1)</td><td>0.80 (1)</td><td>0.47 (1)</td></tr><tr><td>8.7 (2)</td><td>0.80 (2)</td><td>0.48 (2)</td></tr><tr><td>7.4 (4)</td><td>0.68 (4)</td><td>0.58 (4)</td></tr><tr><td>8.2 (6)</td><td>0.86 (6)</td><td>0.50 (6)</td></tr><tr><td>10 (8)</td><td>0.81 (8)</td><td>0.44 (8)</td></tr></table>	Delivery (%)	25%Dilution	50% Dilution	23 (0)	0.91 (0)	0.64 (0)	11 (1)	0.80 (1)	0.47 (1)	8.7 (2)	0.80 (2)	0.48 (2)	7.4 (4)	0.68 (4)	0.58 (4)	8.2 (6)	0.86 (6)	0.50 (6)	10 (8)	0.81 (8)	0.44 (8)			Mathis, 1983
Delivery (%)	25%Dilution	50% Dilution																										
23 (0)	0.91 (0)	0.64 (0)																										
11 (1)	0.80 (1)	0.47 (1)																										
8.7 (2)	0.80 (2)	0.48 (2)																										
7.4 (4)	0.68 (4)	0.58 (4)																										
8.2 (6)	0.86 (6)	0.50 (6)																										
10 (8)	0.81 (8)	0.44 (8)																										

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Ethyl- <i>n</i> -caprylate (in α -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Ethylcellulose	5%	Reconstituted tobacco sheet	Incorporation of 5% ethylcellulose during the slurry process (aqueous and nonaqueous: 80:20 toluene/methanol (v/v) $\Rightarrow$ preparation of cigarettes	n.d.	n.d.	<i>Nonaqueous solvent sheet</i> B[a]P: 1.2 ppm (9.1% $\nearrow$) phenol: 0.4% (20% $\nearrow$) nicotine: - <i>Aqueous solvent sheet</i> B[a]P: 0.9 ppm (18.2% $\nearrow$) phenol: 0.4% (20% $\nearrow$) nicotine: 5.9% (4.8% $\nearrow$)	Halter and Ito, 1972
Ethylene glycol	3%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	B[a]P (in smoke of 500 g tobacco): 2.4 μ g (56% $\nearrow$)	Bentley and Burgan, 1960
Ethylene glycol	3%	Tobacco	n.r.	n.d.	n.d.	B[a]P (per 100 treated cigarettes): 1.2 μ g (50% $\nearrow$)	Pyriki et al., 1965
Ethylene glycol	10%	Flue-cured tobacco	Impregnation with an aqueous solution	n.d.	n.d.	dry TPM: 1.14 mg/5 cig (30.9% $\nearrow$)	Bilimoria and Nisbet, 1975
Ethylene glycol	3%	Tobacco	n.r.	Estimated transfer rate of ethylene glycol into the smoke: $\sim$ 40%	n.d.	n.d.	Reif, 1949
Eugenol	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 22% $\nearrow$ "tar": 22% $\nearrow$ nicotine: 10% $\nearrow$ phenol: 21% $\nearrow$ o-cresol: 2% $\nearrow$ m-, p-cresol: 17% $\nearrow$ B[a]P: 34% $\nearrow$	Burton and Benner, 1972
Formic acid	33 mg/cig	Cigarette	Syringe injection	n.d.	n.d.	<i>Non-filter cigarettes</i> TPM: 32 mg/cig (32.2% $\nearrow$) phenols: 289 μg/cig (54.6% $\nearrow$) <i>Cigarettes + CH-filter</i> TPM: 18 mg/cig (17.7% $\nearrow$) phenols: 64 μg/cig (3% $\nearrow$) <i>Cigarettes + CA-filter</i> TPM: 25.5 mg/cig (50% $\nearrow$) phenols: 76 μg/cig (23.2% $\nearrow$)	Lakritz et al., 1969
Formic acid	33 mg/cig	Cigarette	Injection	n.d.	n.d.	<i>Non-filter cigarettes</i> TPM: 32 mg/cig (32.2% $\nearrow$) pyridine: 9.7 μg/cig (64.7% $\nearrow$) nicotine: 2.34 mg/cig (35.3% $\nearrow$) smoke pH: 4.1 (26.6% $\nearrow$)	Stedman et al., 1969

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Formic acid (33 mg/cig, contd.)						<i>Cigarettes + CH-filter</i> TPM: 18 mg/cig (17.6% ↗) pyridine: 3.7 µg/cig (32.9% ↘) nicotine: 1.2 mg/cig (2.6% ↗) smoke-pH: 4.9 (19.7% ↘) <i>Cigarettes + CA-filter</i> TPM: 25.5 mg/cig (45.7% ↗) pyridine: 7.7 µg/cig (58.4% ↘) nicotine: 1.82 mg/cig (55.6% ↗) smoke pH: 4.4 (24.1% ↘)
Fructose	12.8%	Burley tobacco	Spraying with aqueous sugar solutions	n.d.	n.d.	TPM: 30 mg/cig (11.8% ↘) alkaloids: 2.2 mg/cig (33.4% ↘) carbonyls: 4.4 mg/cig (10% ↗) volatile carbonyls: 2.2 mg/cig (15.8% ↗) volatile aldehydes: 0.53 mg/cig (11.7% ↘) 2-furfural: 89 µg/cig (67.9% ↗) total acids: 2.67 mg/cig (13.6% ↗) volatile acids: 1.23 mg/cig (17.1% ↗)
Fructose	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 4% ↗ "tar": 4% ↗ nicotine: 5% ↘ phenol: 14% ↗ o-cresol: 39% ↗ m-, p-cresol: 19% ↗ B[a]P: 27% ↘
Fructose	4.4 × 10 ⁷ dpm of ¹⁴ C-fructose/g tobacco	Cigarette	Syringe addition of ¹⁴ C-fructose 10 mg/4 mL H ₂ O ⇒ preparation of cigarettes	n.d.	Conversion of ¹⁴C-fructose in tobacco to ¹⁴C-catechol in MSS: 0.008%; estim. min. contribution of fructose to MSS-catechol: 1.4%; estim. min. contribution of fructose, glucose and sucrose to MSS-catechol: 4%	n.d.
Furan-acetylene-dicarboxylic acid	46.4% in adduct 2 g/100 g tobacco	Tobacco	Spraying	n.d.	furan: 1.08 mg/cig transfer rate: 11.6%	n.d.
						Robb <i>et al.</i> , 1964

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Gallic acid	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 5% ↗ "tar": 5% ↗ nicotine: 14% ↗ phenol: 70% ↗ o-cresol: 28% ↗ m-, p-cresol: 8% ↗ B[a]P: 39% ↗	Burton and Benner, 1972
Galvinoxyl	2%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 14% ↗ "tar": 12.1% ↗ nicotine: 42.9% ↗ phenol: 28.2% ↗ o-cresol: 12% ↗ m-, p-cresol: 12.4% ↗ B[a]P: 17.9% ↗	Burton and Benner, 1972
Geraniol (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Geranyl acetone	n.r.	Cigarette	n.r.	Flavour constituents in smoke decreased to different extents when ventilation was increased	n.r.	Reduction of CO and "tar" deliveries with increasing ventilation	Jing and Xian, 1999 (A)
Glucose	29 μ Ci/cig 14 C-D-glucose	Burley tobacco	Spraying of an alcoholic solution of 14 C-D-glucose (5.4 mCi/mol)	n.r.	% of 14 C in glucose: 0.05 acetaldehyde: 0.01 furan: 0.01 propionaldehyde: < 0.01 acetone: 0.08 acrolein: < 0.01 2-methylfuran: 0.02 2-butanone: 0.02 benzene: < 0.005 3-buten-2-one: < 0.01 2,5-dimethylfuran: 0.03 acetonitrile: 0.03 2,3-butanedione: 0.01 crotonaldehyde: < 0.01	n.d.	Gager et al., 1971b
Glucose	16.1%	Air-cured blend	Spraying with aqueous sugar solutions (14 C-nicotine was used)	n.d.	n.d.	Average nicotine directed into MSS: air-cured cigarette: 42.9% air-cured cigarette + glucose: 36.7%	Thornton and Massey, 1975
Glucose	10.5% or 16.8%	Burley tobacco	Spraying with aqueous sugar solutions	n.d.	n.d.	10.5% TPM: 31 mg/cig (8.8% ↗) alkaloids: 2.59 mg/cig (22% ↗) carbonyls: 4.2 mg/cig (5% ↗) volatile carbonyls: 2.0 mg/cig (5.3% ↗) volatile aldehydes: 0.5 mg/cig (16.7% ↗) 2-furfural: 67 μ g/cig (26.4% ↗) total acids: 2.49 mg/cig (6% ↗) volatile acids: 1.11 mg/cig (5.7% ↗)	Thornton and Massey, 1975

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Glucose (10.5% or 16.8%, contd.)						16.8% TPM: 32 mg/cig (5.9% ↘) alkaloids: 2.16 mg/cig (34.9% ↘) carbonyls: 4.3 mg/cig (7.5% ↗) volatile carbonyls: 2.1 mg/cig (10.5% ↗) volatile aldehydes: 0.54 mg/cig (10% ↘) 2-furfural: 80 µg/cig (50.9% ↗) total acids: 2.49 mg/cig (6% ↗) volatile acids: 1.16 mg/cig (10.5% ↗)	
Glucose	0–8%	Powder (0.1 g) of extracted cigarette tobacco	Mixture with leaf powder or powder from extracted cigarettes	n.r.	n.d.	No alteration of alkylating activity by glucose when pyrolysed in air	Crosthwaite <i>et al.</i> , 1979
Glucose	29 µCi/cig ¹⁴ C-D-glucose	Burley tobacco	Spraying of an alcoholic solution of ¹⁴ C-D-glucose- (5.4 mCi/mol)	~ 0.5% of D-glucose	Gas phase CO ₂ : 2.7% tot. act. CO: 1.7% tot. act. Organic components 0.3% tot. act. TPM: 6.4% tot. act.	n.d.	Gager <i>et al.</i> , 1971a
Glucose	Activity: 2.21 × 10 ⁷ cpm	Tobacco	Impregnation with an ethanol-water solution containing 5.12 × 10 ⁵ cpm/mL of ¹⁴ C-labelled glucose	n.r.	Glucose conversion into phenol 0.0213%; total phenols in flue-cured tobacco: 41% (estim.)	n.d.	Bell <i>et al.</i> , 1966
Glucose	1454 × 10 ³ cpm/cig	Cigarette	Hypodermic syringe injection of 80 µL of ¹⁴ C-glucose containing solutions	n.d.	Activity recovered particulate: 4.9% vapour: 5.4% butt: 45.3%	n.d.	Thornton and Valentine, 1968
Glutamic acid	5% (w/w)	Cigarette ("bright yellow" or "Matsukawa" tobacco)	n.r.	n.d.	n.d.	"Bright Yellow" acrylonitrile: - acetoneitrile: 15.7 µg/puff (180% ↗) isobutyronitrile: 1.7 µg/puff (160% ↗) propionitrile: 6.0 µg/puff (210% ↗) n-butyronitrile: 1.4 µg/puff (160% ↗) "Matsukawa" acrylonitrile: 0.9 µg/puff (30% ↘) acetoneitrile: 25.7 µg/puff (130% ↗) isobutyronitrile: 2.3 µg/puff (10% ↘) propionitrile: 8.1 µg/puff (100% ↗) n-butyronitrile: 2.9 µg/puff (320% ↗)	Kaburaki <i>et al.</i> , 1969

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Glycerol	2 and 3%	Tobacco	Diluted with water by spraying	n.d.	n.d.	2%: nicotine: 1.2 mg/cig (0.8% ↗) "tar": 27.4 mg/cig (8.7% ↗) CO: 16.7 mg/cig (12.1% ↗) 3%: nicotine: 1.24 mg/cig (4.2% ↗) "tar": 28 mg/cig (11.1% ↗) CO: 16.9 mg/cig (13.4% ↗) n.d.	Stoilova <i>et al.</i> , 1994
Glycerol	4.39% on tobacco 0.35–8.13% on tobacco	Filter cigarettes	n.r.	70 mm test cigarettes 4.98 mg/g tobacco ⇒ 8.9% transfer 85 mm filter cigarettes 1.3–4.98 mg/g tobacco ⇒ 4.8–5.2% transfer	n.d.	n.d.	Laurene <i>et al.</i> , 1965
Glycerol	3%	Tobacco	Addition to dried tobacco	n.d.	n.d.	nicotine: 3.03–3.28 mg/cig (1.7–4.1% ↗) TPM: 47.2 mg/cig (4.7% ↗) dry condensate: 42 mg/cig (↔)	Smit, 1970
Glycerol	3%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	B[a]P (in smoke of 500 g tobacco): 2.1 µg (62% ↗)	Bentley and Burgan, 1960
Glycerol	3.4 and 10%	Flue-cured tobacco and flue-cured blend	Impregnation with an aqueous solution	n.d.	n.d.	TPM: tobacco + 10%: 163 mg/5 cig (1.2% ↗) blend + 3.4%: 121 mg/5 cig (7.1% ↗)	Bilimoria and Nisbet, 1975
Glycerol	40% carbon content	Cigarette	Spraying of cigarettes with labelled ¹⁴ C-glycerol	n.d.	Carbon ⇒ MSS: gas phase: 8.6% TPM: 22.0%	n.d.	Jenkins <i>et al.</i> , 1980
Glycerol	2.95% (w/w)	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of cigarettes (SEB III)	n.d.	n.d.	Concentration/cigarette TPM: 31.6 mg/cig (1.1% ↗) "tar": 27.1 mg/cig (0.8% ↗) water: 2.69 mg/cig (3.9% ↗) nicotine: 1.8 mg/cig (5.8% ↗) phenol: 164 µg/cig (15.7% ↗) acetaldehyde: 1.176 mg/cig (7.9% ↗) acrolein: 108 µg/cig (7.9% ↗) isoprene: 460 µg/cig (16.2% ↗) HCN: 338 µg/cig (2.3% ↗) formaldehyde: 34 µg/cig (5.3% ↗) NO _x : 436 µg/cig (3.8% ↗) CO: 16.1 mL/cig (1.3% ↗) CO ₂ : 32.6 mL/cig (5.0% ↗)	NCI, Report No. 3, 1977

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Glycerol (2.95%, contd.)						Concentration/g dry condensate indole: 463 µg/g (29.4% ↗) skatole: 315 µg/g (6.5% ↗) B[a]A: 1.41 µg/g (6.0% ↗) B[a]P: 1.02 µg/g (5.6% ↗) o-cresol: 0.70 mg/g (2.8% ↗) m-, p-cresol: 1.93 mg/g (6.8% ↗) tot. w-acids: 2.24 mg/g (3.9% ↗) fatty acids: 21.61 mg/g (0.5% ↗) OLL-acids: 12.92 mg/g (1.5% ↗) palmitic acid: 6.60 mg/g (0.3% ↗) stearic acid: 2.09 mg/g (12.9% ↗) catechol: 5.18 mg/g (11.3% ↗) n.d.	Ishiguro <i>et al.</i> , 1979
Glycerol	72.7–686 µg/cig rod smoked	Tobacco	Manufacture of cigarettes from different treated tobacco types	Approximately 20% of glycerin in tobacco was transferred to mainstream smoke	n.d.		
Glycerol	3%	Tobacco	n.r.	n.d.	n.d.	B[a]P (per 100 treated cigarettes): 1.1 µg (37.5% ↗)	Pyriki <i>et al.</i> , 1965
Glycerol	n.r.	Cigarette	n.r.	Transfer rates for propylene glycol were more affected by filter ventilation than were those for glycerol	n.r.	n.r.	Cook <i>et al.</i> , 1999 (A)
Glycerol	3.3 and 6.1% (w/w)	Tobacco	Spraying of an alcoholic glycerol solution	n.d.	n.d.	3.3%: B[a]P: 3.48 µg/100 cig (3.9% ↗) "tar": 31.8 mg/cig (2.3% ↗) nicotine: 2.06 mg/cig (5.5% ↗) 6.1%: B[a]P: 3.51 µg/100 cig (4.8% ↗) "tar": 30.6 mg/cig (1.6% ↗) nicotine: 2.02 mg/cig (7.3% ↗)	de Souza and Scherbak, 1964
Glycerol	3.35% (43.3 mg/cig)	Cigarette	Addition during casing of cigarette tobacco	plain cigarette: 3.46 mg/cig ⇒ transfer rate 14% filter cigarette: 3.71 mg/cig ⇒ transfer rate 12%	n.d.	TPM: 67 mg/cig (13.9% ↗) polyol: 6.95 mg/cig (15.7% ↗) nicotine: 6.1 mg/cig (2.3% ↗) volatile acids: 2.22 mg/cig (22.9% ↗) acetaldehyde: 0.93 mg/cig (14.8% ↗) 2,4-DNP: 8.14 mg/cig (1.3% ↗) propionaldehyde: 0.05 mg/cig (25% ↗) acetone: 0.1 mg/cig (25% ↗)	Kobashi <i>et al.</i> , 1965

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Glycine	N added as glycine: 2%	Tobacco	Spraying of an aqueous solution with labelled ^{15}N glycine	n.r.	HCN: 82 $\mu\text{g}/\text{cig}$ ^{15}N	n.d.	Johnson <i>et al.</i> , 1973
Glycosylamine	5% (w/w)	Tobacco	Spraying of an aqueous solution (50%) onto tobacco filler	n.r.	flavour ammonia pyrazine	"tar": 8 mg/cig	Cox <i>et al.</i> , 1987 (P)
Glycyrrhetinic acid	10 mg/g tobacco shreds	Tobacco (flue-cured, burley, Oriental, blended tobacco)	n.r.	<i>Non-filter cigarettes:</i> 0.108 mg/cig $\Rightarrow$ 2.53% transfer rate <i>Filter cigarettes:</i> 0.098 mg/cig $\Rightarrow$ 2.3% transfer rate	n.d.	n.d.	Sakagami, 1973
Glycyrrhizic acid	10 mg/g tobacco shreds	Tobacco (flue-cured, burley, Oriental, blended tobacco)	n.r.	n.d.	<i>Non-filter cigarettes:</i> 0.108 mg/cig glycyrrhetinic acid $\Rightarrow$ 2.29% <i>Filter cigarettes:</i> 0.097 mg/cig glycyrrhetinic acid $\Rightarrow$ 2.07%	n.d.	Sakagami, 1973
Hexadien-(2,4)-al (in α -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Hexadien-(2,4)-al (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
H ₂ -1 catalyst	10%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.	<i>Fifth puff (35 mL)</i> H ₂ : 0.85 mol% (3.7% $\nearrow$) O ₂ : 14.24 mol% (1.6% $\nearrow$) CO: 1.9 mol% (6.7% $\nearrow$) CO ₂ : 5.18 mol% (5.2% $\nearrow$) NO + NO ₂ : 20.3 μg (33.6% $\nearrow$) N ₂ O: < 1 μg ($\rightarrow$) HCN: 16.5 μg (25% $\nearrow$) H ₂ S: 1.7 μg (13.3% $\nearrow$) SO ₂ : 2.6 μg (36.8% $\nearrow$) CH ₄ : 79.9 μg (14.3% $\nearrow$) C ₂ H ₆ : 26.5 μg (15.7% $\nearrow$) ethylene: 11.8 μg (10.3% $\nearrow$) acetaldehyde: 40.3 μg (14.1% $\nearrow$) acetone: 22.8 μg (15.6% $\nearrow$) acetonitrile: 9.1 μg (28.9% $\nearrow$) acrolein: 5.8 μg (1.8% $\nearrow$) formaldehyde: 5.2 μg (6.1% $\nearrow$) methanol + methyl chloride + methyl acetylene: 17.2 μg (28.6% $\nearrow$)	Terrell and Schmeltz, 1970

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)	
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS		
Indole	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 47.4% ↗ "tar": 50.6% ↗ nicotine: 2.9% ↗ phenol: 1.4% ↗ o-cresol: 20% ↗ m-, p-cresol: 2.6% ↗ B[a]P: 30.8% ↗	Burton and Benner, 1972	
β-Ionone	n.r.	Cigarette	n.r.	Flavour constituents in smoke decreased to different extents when ventilation was increased	n.r.	Reduction of CO and "tar" deliveries with increasing ventilation	Jing and Xian, 1999 (A)	
Isoamyl benzoate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of isoamyl benzoate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 55 (0) 0.92 (0) 0.68 (0) 47 (1) 0.94 (1) 0.64 (1) 42 (2) 0.81 (2) 0.59 (2) 36 (4) 0.57 (4) 0.46 (4) 34 (6) 0.67 (6) 0.42 (6) 35 (8) 0.58 (8) 0.34 (8)	n.d.	n.d.	n.d.	Mathis, 1983
Isoamyl cinnamate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of isoamyl cinnamate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 29 (0) 0.90 (0) 0.68 (0) 21 (1) 0.77 (1) 0.46 (1) 20 (2) 0.71 (2) 0.47 (2) 13 (4) 0.85 (4) 0.52 (4) 14 (6) 1.00 (6) 0.58 (6) 21 (8) 0.49 (8) 0.30 (8)	n.d.	n.d.	n.d.	Mathis, 1983
Isoamyl isovalerate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of isoamyl isovalerate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 40 (0) 0.46 (0) 0.57 (0) 20 (1) — 0.61 (1) 20 (2) 0.45 (2) 0.47 (2) 21 (4) 0.52 (4) 0.50 (4) 22 (6) 0.92 (6) 0.62 (6) 17 (8) 0.97 (8) 0.51 (8)	n.d.	n.d.	n.d.	Mathis, 1983

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)		
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products		Influence on MSS	
Isoamyl isovalerate	44 µCi/cig (142 µg)	Cigarette	Manual syringe injection of cigarettes with ¹⁴ C-labelled isoamyl isovalerate (54 mCi/mmol)	TPM: 11.7% vapour phase: 6.7%	Extent of decomposition: 0%	n.d.	Green <i>et al.</i> , 1989	
Isoamyl isovalerate	1 mg	Capillary tube (modelling cigarette combustion)	No application to tobacco	Predicted transfer of isoamyl isovale-rate: 99.6% (200 °C, 2% and 10% O ₂)	<i>Further combustion products:</i> isobutyl isovalerate: 0.4%	n.d.	Stotesbury <i>et al.</i> , 1999	
Isoamyl phenylacetate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of isoamyl phenylacetate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 51 (0) 0.90 (0) 0.72 (0) 40 (1) 0.92 (1) 0.55 (1) 36 (2) 0.82 (2) 0.60 (2) 27 (4) 0.57 (4) 0.38 (4) 26 (6) 0.76 (6) 0.53 (6) 26 (8) 0.65 (8) 0.38 (8)	n.d.	Isoprene delivery: control (expanded stems): 91 µg/cig expanded stems + polymer: 182 µg/cig commercial cigarette: 589 µg/cig	n.d.	Van Aukén <i>et al.</i> , 1979 (P)
Lactic acid	100 mg/cig	Cigarettes	Syringe injection	n.d.	n.d.	<i>Non-filter cigarettes</i> TPM: 29.9 mg/cig (21.1% ↗) formic acid: 75 µg/cig (35.3% ↗) acetic acid: 248 µg/cig (39.8% ↗) <i>Cigarettes + CH-filter</i> TPM: 21.9 mg/cig (16.5% ↗) formic acid: 46 µg/cig (37% ↗) acetic acid: 72 µg/cig (67.9% ↗) <i>Cigarettes + CA-filter</i> TPM: 15.6 mg/cig (8.3% ↗) formic acid: 22 µg/cig (57.7% ↗) acetic acid: 135 µg/cig (41% ↗)	Lakritz <i>et al.</i> , 1969	

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Lead borate (glass)	10%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.	<i>Fifth puff (35 mL)</i> H ₂ : 0.65 mol% (20.7% ↗) O ₂ : 15.12 mol% (7.1% ↗) CO: 1.36 mol% (25.6% ↗) CO ₂ : 4.91 mol% (10.1% ↗) NO + NO ₂ : 22.8 µg (50% ↗) N ₂ O: < 1 µg (↔) HCN: 18.7 µg (41.6% ↗) H ₂ S: 0.2 µg (86.7% ↗) SO ₂ : 1.8 µg (5.3% ↗) CH ₄ : 57.4 µg (17.9% ↗) C ₂ H ₆ : 19.5 µg (14.8% ↗) ethylene: 10.1 µg (5.6% ↗) acetaldehyde: 37.4 µg (20.3% ↗) acetone: 21.9 µg (18.9% ↗) acetonitrile: 10 µg (21.9% ↗) acrolein: 5.5 µg (3.5% ↗) formaldehyde: 5.6 µg (14.3% ↗) methanol + methyl chloride + methyl acetylene: 17.1 µg (29% ↗)
Lead nitrate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke Bentley and Burgan, 1960
D-Limonene (3.1% in α-cyclodextrine)	4%	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	Bavley and Robb, 1969 (P)
D-Limonene (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	Bavley and Robb, 1969 (P)
D-Limonene (in tri- <i>o</i> -thymoid)	1%	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	Bavley and Robb, 1969(P)
Linalool (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	Bavley and Robb, 1969 (P)
Linalool (in γ-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	Bavley and Robb, 1969 (P)
Lithium nitrate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 19.4% ↗ "tar": 15.7% ↗ nicotine: 67.6% ↗ phenol: 43.6% ↗ o-cresol: 35% ↗ <i>m</i> -, <i>p</i> -cresol: 54.8% ↗ B[a]P: 60.7% ↗ Burton and Benner, 1972
Magnesium acetate	n.r.	Tobacco	Treatment with 2% aqueous solution	n.d.	n.d.	"tar": 28.1 mg/cig (2.8% ↗) Aksu, 1969

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)	
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products		
Magnesium carbonate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 20.1% ↗ "tar": 22.1% ↗ nicotine: 3.6% ↗ phenol: 7% ↗ o-cresol: 60% ↗ m-, p-cresol: 19.2% ↗ B[a]P: 7.7% ↗	Burton and Benner, 1972
Magnesium carbonate (basic)	10%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.	<i>Fifth puff (35 mL)</i> H ₂ : 1.42 mol% (73.2% ↗) O ₂ : 12.82 mol% (8.5% ↗) CO: 2.88 mol% (61.8% ↗) CO ₂ : 6.97 mol% (16.9% ↗) NO + NO ₂ : 23.8 µg (56.6% ↗) N ₂ O: <1 µg (↔) HCN: 22.4 µg (69.7% ↗) H ₂ S: 3.2 µg (113.3% ↗) SO ₂ : 2.6 µg (36.8% ↗) CH ₄ : 119.9 µg (71.5% ↗) C ₂ H ₆ : 36.5 µg (59.4% ↗) ethylene: 18.8 µg (75.7% ↗) acetaldehyde: 68.5 µg (46.1% ↗) acetone: 33.7 µg (24.8% ↗) acetonitrile: 13.4 µg (4.7% ↗) acrolein: 9.6 µg (68.4% ↗) formaldehyde: 2.4 µg (51% ↗) methanol + methyl chloride + methyl acetylene: 36 µg (49.4% ↗)	Terrell and Schmelzt, 1970
Magnesium nitrate	0.55%	Reconstituted tobacco sheet	Incorporation into a reconstituted tobacco sheet ⇒ manufacture of cigarettes	n.d.	n.d.	PAH concentrations in smoke (infra-red arbitrary units in % of control): 78% ⇒ 22% ↗	Norman and Bryant, 1975 (P)
Magnesium nitrate	0.47% nitrate to the casings	Tobacco	Casing formulation with nitrate salt	n.d.	n.d.	1.895 mg PAH/g dry smoke (15.6% ↗) in comparison to the average of 4 controls	Collins et al., 1981 (P)
Magnesium nitrate	5.72%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of cigarettes (SEB III)	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 33.39 mg/cig (5.7% ↗) "tar": 27.99 mg/cig (3.3% ↗) water: 3.77 mg/cig (40.1% ↗) nicotine: 1.63 mg/cig (9.4% ↗) phenol: 199.92 µg/cig (21.9% ↗) acetaldehyde: 1.32 mg/cig (12.2% ↗) acrolein: 133.38 µg/cig (23.5% ↗) isoprene: 546.25 µg/cig (18.8% ↗) HCN: 510.5 µg/cig (51.0% ↗) formaldehyde: 34.5 µg/cig (1.5% ↗) NO ₂ : 1379 µg/cig (216.3% ↗) CO: 17.65 mL/cig (9.6% ↗) CO ₂ : 38.25 mL/cig (17.3% ↗)	NCI, Report No. 3, 1977

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	
Magnesium nitrate (5.7%, contd.)					Concentration/g dry condensate indole: 439.8 µg/g (5.0% ↗) skatole: 303.2 µg/g (3.7% ↗) B[a]A: 1.43 µg/g (1.4% ↗) B[a]P: 1.21 µg/g (18.6% ↗) o-cresol: 0.52 mg/g (25.7% ↗) m-, p-cresol: 1.61 mg/g (16.6% ↗) tot. w-acids: 2.12 mg/g (12.4% ↗) fatty acids: 21.25 mg/g (1.7% ↗) OLL-acids: 12.83mg/g (0.7% ↗) palmitic acid: 6.23 mg/g (5.6% ↗) stearic acid: 2.10 mg/g (0.5% ↗) catechol: 4.74 mg/g (8.5% ↗) glycerol: 72.2 mg/g (7.5% ↗) n.d.	Thornton and Valentine, 1968
Maleic anhydride	603 × 10 ³ cpm/cig	Cigarettes	Hypodermic syringe injection of 80 µL of maleic anhydride-1,4- ¹⁴ C containing solutions	n.d.	Activity recovered particulate: 2.1% vapour: 15.0% butt: 27.6%	
Manganese nitrate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	Burton and Benner, 1972
Megastigmatrienone released from: 3-oxo- α -ionol ethyl carbonate	0.002%	Cigarette	Manufacture of treated and untreated cigarettes	n.d.	Thermal elimination of the precursor producing megastigmatrienone	Yang <i>et al.</i> , 2001
Menthol	3.6 mg	Cigarette filter	Mixture of a menthol (80%)/ethanol (20%) -solution with filter material (Poropak Q)	fresh: 0.53 mg/cig transfer of menthol: 14.7% aged: 0.38 mg/cig transfer of menthol: 10.6% carbon filter: 0.04 mg/cig transfer of menthol: 1.1%	n.d.	
Menthol released from: <i>Mentha arvensis</i>	10%	Tobacco	Mixture of dried mint leaves (shredded leaves, containing 1.56% menthol) and Virginia tobacco	Menthol delivery of cigarettes: 16%	n.d.	BAT Co Ltd, 1978 (Research disclosure)
Menthol (4.6 and 5% in tri-o-thymoid)	1%	Tobacco	Spraying	n.d.	150–200 µg/cig (sampled on CF) estim. transf.: 33–43%	Bavley and Robb, 1969 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Menthol (3.6% in α -cyclodextrine)	0.6%	Tobacco	Spraying	n.d.	35–50 μ g/cig (sampled on CF) estim. transf.: 16–23%	n.d.	Bavley and Robb, 1969 (P)
Menthol (6.42% in β -cyclodextrine)	2.5%	Tobacco	Spraying	n.d.	130–160 μ g/cig (sampled on CF) estim. transf.: 8.1–10%	n.d.	Bavley and Robb, 1969 (P)
Menthol (in γ -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Menthol	26% (w/w)	Tobacco (cigarette T) or filter tow (cigarette F)	Tow of the filter was bonded with a 55/45 triacetin/polyethylene glycol blend containing menthol	Cigarette F: 3 d storage: 0.92 mg $\Rightarrow$ 49% 28 d storage: 0.59 mg $\Rightarrow$ 31% Cigarette T: 3 d storage: 0.48 mg $\Rightarrow$ 20% 28 d storage: 0.45 mg $\Rightarrow$ 19%	n.d.	n.d.	Curran, 1972
Menthol	0.013–3.2 mg/cig	Cigarette, samples A–H: different cigarette brands	n.r.	Menthol in smoke and transfer rate Sample A: 0.63 mg/cig $\Rightarrow$ 29.9% Sample B: 0.56 mg/cig $\Rightarrow$ 28.7% Sample C (100 mm Cig): 0.49 mg/cig $\Rightarrow$ 31.0% Sample D: 0.42 mg/cig $\Rightarrow$ 24.7% Sample E: 0.38 mg/cig $\Rightarrow$ 29.5% Sample F: 0.31 mg/cig $\Rightarrow$ 27.5% Sample G (perforation): 0.23 mg/cig $\Rightarrow$ 18.7% Sample H: 0.31 mg/cig $\Rightarrow$ 31.0% Sample J: 0.019 mg/cig $\Rightarrow$ 24.1% Menthone in smoke of samples B and H 2–4% of menthol	n.d.	n.d.	Brozinski et al., 1972
Menthol	2 mg/cig	Tobacco	Menthol: n.r.; filter additives by brush applicator system	Transfer rate of menthol: 5% triacetin: 0.39 mg/cig (14.7% $\rightarrow$) 8% triacetin: 0.36 mg/cig (5.9% $\rightarrow$) 5% triethylene glycol diacetate (TGD): 0.33 mg/cig (2.9% $\rightarrow$) 8% TGD: 0.30 mg/cig (11.8% $\rightarrow$) 6% glycerol: 0.30 mg/cig (16.7% $\rightarrow$) 10% glycerol: 0.30 mg/cig (16.7% $\rightarrow$) 6% 1,2-propanediol: 0.29 mg/cig (19.4% $\rightarrow$) 10% 1,2-propanediol: 0.27 mg/cig (25% $\rightarrow$) n.d.	n.d.	n.d.	Curran, 1975
Menthol released from poly(α -styryl- β -menthyl carbonate)	2.2% (w/w) (tobacco)	Tobacco	Spraying of a cyclohexane solution containing the flavour precursor	n.d.	Release of menthol: 0.23 mg/cig Release of menthol after storage: 0.24 mg/cig	n.d.	Grubbs et al., 1978 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Menthol released from poly(α -methylvinyl Δ -menthyl carbonate)	1.7%, 1.74% or 2.37% (w/w) (tobacco)	Tobacco	Spraying of a cyclohexane solution containing the flavour precursor	n.d.	1.7%; 820 mg: 0.24 mg/cig 1.74%; 780 mg: 0.36 mg/cig 2.37%; 820 mg: 0.44 mg/cig	n.d.	Grubbs <i>et al.</i> , 1978 (P)
Menthol	Unlabelled menthol: 3 mg/cig ^{14}C -menthol: 1.1 μCi	Non-filtered cigarette	Syringe injection of labelled ^{14}C -menthol	Percentage of total mainstream activity: menthol: 98.9%	Percentage of total mainstream activity: CO_2 : 0.1% menthane: 0.2% menthone: 0.4%	gas phase: 0.01 $\mu\text{Ci} \Rightarrow$ 1% TPM: 0.29 $\mu\text{Ci} \Rightarrow$ 27.9% total activity: 28.9%	Jenkins <i>et al.</i> , 1970b
Menthol	n.r.	Cigarette	n.r.	Flavour constituents in smoke decreased to different extents when ventilation was increased	n.r.	Reduction of CO and "tar" deliveries with increasing ventilation	Jing and Xian, 1999 (A)
Menthol	n.r.	Cigarette	n.r.	n.r.	n.r.	n.r.	Cook <i>et al.</i> , 1999 (A)
Menthol	n.r.	n.r.	n.r.	Sample A: 0.39–0.43 mg/cig Sample B: 0.48–0.50 mg/cig Sample C: 0.29–0.31 mg/cig Sample D: 0.21–0.23 mg/cig	n.d.	n.d.	Lyerly, 1967
Menthol	1.2–2.56 mg (four different concentrations)	Filter	Solution of menthol in chloroform applied to four brands	menthol in MSS: 0.35–0.58 mg/cig menthol in cigarette: 1.6–2.2 mg/cig transfer rate: 22–26%	n.d.	n.d.	Mitchell <i>et al.</i> , 1963
Menthol	Amount of menthol on the plug wrap 5.9 mg	Cigarette plug wrap	Menthol was solubilized in ethanol and mixed with triacetin	Transfer of menthol into the smoke on a puff by puff basis (experimental, no storage): 1. Puff $\Rightarrow$ 0.04 mg 2. Puff $\Rightarrow$ 0.04 mg 3. Puff $\Rightarrow$ 0.04 mg 4. Puff $\Rightarrow$ 0.04 mg 5. Puff $\Rightarrow$ 0.04 mg 6. Puff $\Rightarrow$ 0.05 mg 7. Puff $\Rightarrow$ 0.06 mg 8. Puff $\Rightarrow$ 0.09 mg 9. Puff $\Rightarrow$ 0.15 mg menthol in all puffs: 0.68 mg $\Rightarrow$ transfer rate: 11.5% menthol delivery under different storage conditions: 0.26–0.73 mg $\Rightarrow$ 4.4–12.4%	n.d.	n.d.	Nichols <i>et al.</i> , 1987 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Menthol	2.7 mg on the finished cigarette	Tobacco or filter tow	Prior to final cigarette assembly menthol application to cigarette F (from triethylene glycol diacetate/polyethylene glycol) and cigarette T (from ethanolic solution)	Highest menthol transfer when most of the menthol is on the filter ~ 30% High transfer when most of the menthol is on the tobacco ~ 20% When 70% of menthol is on the tobacco or 60% of the menthol is on the filter → 16% transfer to MSS	n.d.	n.d.	Riehl <i>et al.</i> , 1973
Menthol	10%	Conventional filter or a porous, hydrophilic acrylate or methacrylate polymer	Impregnation with an alcoholic solution (10%)	n.d.	n.d.	Polymeric filter + menthol TPM: 7.7 mg/cig (80.0% ↗) "tar": 6.8 mg/cig (77.5% ↗) nicotine: 0.1 mg/cig (93.7% ↗)	Shepherd and Gould, 1968 (P)
Menthol	Nine formulations (A-I) FF-M: 0.12–1.05% FFLT-M: 0.16–0.83% ULT-M: 0.21–1.31%	Tobacco American blends for FF-M 85 mm FFLT-M 85 mm ULT-M 85 mm	Top dressing with menthol at a constant rate	Release of menthol in smoke ⇒ transfer	n.d.	"Tar" FF-M (A-I): 17.3–18.1 mg/cig FFLT-M (A-I): 8.3–8.9 mg/cig ULT-M (A-I): 5.7–6.4 mg/cig Nicotine FF-M (A-I): 1.23–1.33 mg/cig FFLT-M (A-I): 0.71–0.76 mg/cig ULT-M (A-I): 0.5–0.54 mg/cig TPM FF-M (A-I): 22.1–23.1 mg/cig FFLT-M (A-I): 10.2–11.0 mg/cig ULT-M (A-I): 6.6–7.5 mg/cig	Perfetti and Gordin, 1985

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Menthol (3.6% in α -cyclodextrin)	1.63 g/100 g tobacco	Tobacco	Spraying	n.d.	menthol: 0.05 mg/cig transfer rate: 8.5%	n.d.	Robb <i>et al.</i> , 1964
Menthol (6.4% in β -cyclodextrin)	2.5 g/100 g tobacco	Tobacco	Spraying	n.d.	menthol: 0.14 mg/cig transfer rate: 8.8%	n.d.	Robb <i>et al.</i> , 1964
Menthone (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Methoxymethyl-thiirane	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 29.7% ↗ "tar": 29.5% ↗ nicotine: 32.1% ↗ phenol: 35.9% ↗ o-cresol: 16% ↗ <i>m</i> -, <i>p</i> -cresol: 23.3% ↗ B[a]P: 43.6% ↗	Burton and Benner, 1972
Methyl benzoate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of methyl benzoate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery	n.d.	n.d.	Mathis, 1983
Methyl caprate	480 ppm	Tobacco	Spraying ⇌ manufacture of cigarettes	Delivery (%)	25% Dilution	50% Dilution	Tso, 1975 (P)
				11 (0)	0.82 (0)	0.33 (0)	
				7.2 (1)	0.86 (1)	0.40 (1)	
				10 (2)	0.74 (2)	0.35 (2)	
				11 (4)	0.90 (4)	0.33 (4)	
				12 (6)	1.08 (6)	0.45 (6)	
				13 (8)	0.85 (8)	0.40 (8)	
				n.d.	n.d.	wet TPM: 36.3 mg/cig (17.7% ↗) dry TPM: 32.4 mg/cig (19.2% ↗) nicotine: 3.12 mg/cig (17.9% ↗) volatile phenols: 220 µg/cig (11.7% ↗) B[a]P: 4.19 µg/100 g tobacco (24.1% ↗) B[a]A: 6.24 µg/100 g tobacco (19.1% ↗)	
Methyl cinnamate	69 µCi/cig (227 µg)	Cigarettes	Manual syringe injection of cigarettes with ¹⁴ C-labelled methyl cinnamate (50 mCi/mmol)	TPM: 7.4% vapour phase: 0.2%	Extent of decomposition: 0%	n.d.	Green <i>et al.</i> , 1989

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Methyl cinnamate	0.134 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of methyl cinnamate after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery <i>Delivery (%) 25% Dilution 50% Dilution</i> 33 (0) 0.86 (0) 0.63 (0) 13 (1) 0.91 (1) 0.58 (1) 13 (2) 0.85 (2) 0.52 (2) 12 (4) 0.81 (4) 0.52 (4) 14 (6) 1.00 (6) 0.50 (6) 13 (8) 0.86 (8) 0.48 (8)	n.d.	n.d.	Mathis, 1983
Methyl <i>trans</i> -cinnamate	1 mg	Capillary tube (modelling cigarette combustion)	No application to tobacco	Predicted transfer of methyl cinnamate: 98.8% (400 °C)	<i>Further combustion products</i> 2,6-bis(1,1-dimethyl-ethyl)-4-methylphenol: 0.8% methyl α -methyl-cinnamate: 0.1% 4-methylstyrene: 0.1% 1-methoxyethylbenzene: 0.1% 2-propanone, 1-(4-methoxyphenyl)-oxime: 0.03% 2,6-di- <i>t</i> -butyl-4-methylene-2,5-cyclohexadien-1-one: 0.02% 2-(1-methylethyl)phenol: 0.02% 1-propynylbenzene: 0.02% methyl 2-benzylacrylate: 0.01% indene: 0.01%	n.d.	Statesbury <i>et al.</i> , 1999
Methylsalicylate (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Methylsalicylate (in γ -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Myrcene (in β -cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Neophytadiene	1–3 × 10 ⁶ dpm/cig	Cigarette	Impregnation by the syringe technique with ¹⁴ C-labelled neophytadiene (specific activity 0.274 µCi/µm)	n.d.	Distribution of radioactivity: "tar": 26% volatiles: 2.6% CO ₂ : 6.1% PAH: 0.1% butt: 2.7% ash: 2.4%	n.d.	Schmeltz et al., 1978
Nickel acetate	3.1% nickel acetate × 4H ₂ O	Tobacco	n.r. ⇒ manufacture of treated and untreated cigarettes	n.d.	n.d.	"tar": 28.3 mg/cig (2.1% ↘) B[a]P: 2.5 µg/100 cig (35.1% ↘) phenol: 75 µg/100 cig (23.9% ↘)	Wynder and Hoffmann, 1963
Nickel oxalate	10%	Tobacco	Additive powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.	<i>Fifth puff</i> (35 mL) H ₂ : 2.19 mol% (16.7% ↗) O ₂ : 10.21 mol% (27.1% ↘) CO: 4.13 mol% (132% ↗) CO ₂ : 8.84 mol% (61.9% ↗) NO + NO ₂ : 24.7 µg (62.5% ↗) N ₂ O: < 1 µg (↔) HCN: 23.4 µg (77.3% ↗) H ₂ S: 2.6 µg (73.3% ↗) SO ₂ : 3.1 µg (63.2% ↗) CH ₄ : 124.9 µg (78.7% ↗) C ₂ H ₆ : 43.9 µg (91.7% ↗) ethylene: 23.8 µg (122.4% ↗) acetaldehyde: 66.4 µg (41.6% ↗) acetone: 35.9 µg (33% ↗) acetonitrile: 13.3 µg (3.9% ↗) acrolein: 10.7 µg (87.7% ↗) formaldehyde: 7.1 µg (55.1% ↗) methanol + methyl chloride + methyl acetylene: 33.4 µg (38.6% ↗)	Terrell and Schmeltz, 1970
N-Nitroso-dimethylamine (NDMA)	40.5 µg/cig	Tobacco	NDMA (2.7 mg) was sprayed with a methanol solution	Transfer rate of NDMA from tobacco to the smoke: 20.2%	n.d.	n.d.	Morie and Sloan, 1973
n-Octane (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Orange oil (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Oxo-isophorone	n.r.	Cigarette	n.r.	Flavour constituents in smoke decreased to different extents when ventilation was increased	n.r.	Reduction of CO and "tar" deliveries with increasing ventilation	Jing and Xian, 1999 (A)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Palladium	Sheet: 0.02%	Sheet or tobacco blend (cased), cigarettes	Mixture of sheet or tobacco blend with palladium ⇒ simulation of cigarette pyrolysis	n.d.	n.d.	PAH (from sheet): 59% ↗ cigarettes: 34% ↗	Bryant <i>et al.</i> , 1979 (P)
	Blend: 0.06%					PAH (from blend): 49 and 22% ↗ cigarettes: 29% ↗	
Palladium	470 ppm	Tobacco nitrate: 0.22%	Casing formulation with palladium	n.d.	n.d.	2.072 mg PAH/g dry smoke (7.7% ↗)	Collins <i>et al.</i> , 1981 (P)
Palladium	580 ppm	Tobacco nitrate: 0.59%	Casing formulation with palladium	n.d.	n.d.	1.534 mg PAH/g dry smoke (21.3% ↗)	Collins <i>et al.</i> , 1981 (P)
Palladium	580 ppm	Tobacco nitrate: 0.47%	Casing formulation with palladium	n.d.	n.d.	1.551 mg PAH/g dry smoke (20.4% ↗)	Collins <i>et al.</i> , 1981 (P)
Palladium salts	0.06% (NH ₄) ₂ PdCl ₆ or (NH ₄) ₂ PdCl ₄	Reconstituted tobacco sheet	Incorporation into a reconstituted tobacco sheet ⇒ manufacture of cigarettes	n.d.	n.d.	PAH concentrations in smoke (infra-red arbitrary units in % of control): (NH ₄) ₂ PdCl ₆ : 59% (41% ↗) (NH ₄) ₂ PdCl ₄ : 78% (22% ↗)	Norman and Bryant, 1975 (P)
Palmitic acid	1–3 × 10 ⁶ dpm/cig	Cigarette	Impregnation by the syringe technique with ¹⁴ C-labelled palmitic acid (specific acti-vity 0.205 µCi/µm)	n.d.	Distribution of ¹⁴ C (as fatty acids): "tar": 22.81% volatiles: 0.9% CO ₂ : 1.41% PAH: < 1% butt: 3.5% ash: 0.6%	n.d.	Schmeltz <i>et al.</i> , 1978
Peach concentrate (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Pectin	6%	Tobacco blends	Acid extracts containing 1% pectins were sprayed onto tobacco at a ratio of 6%	n.d.	n.d.	Flavoured cigarette blend: <i>Nitric acid extract</i> nicotine: 1.43 mg/cig (2.1% ↗) "tar": 26.6 mg/cig (2.3% ↗) CO: 20.6 mg/cig (3% ↗) <i>Phosphoric acid extract</i> nicotine: 1.44 mg/cig (1.4% ↗) "tar": 27 mg/cig (3.8% ↗) CO: 20.1 mg/cig (0.5% ↗) <i>Citric acid extract</i> nicotine: 1.45 mg/cig (0.7% ↗) "tar": 26.9 mg/cig (3.5% ↗) CO: 18.9 mg/cig (5.5% ↗)	

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Pectin (6%, contd.)						
Pectin	6%	Tobacco	Different apple extracts with 0.5% pectin and with nitric, phosphoric or citric acid Applied by spraying	n.d.	n.d.	Unflavoured cigarette blend: <i>Nitric acid extract</i> nicotine: 1.19 mg/cig (1.7% ↗) "tar": 25.5 mg/cig (1.2% ↗) CO: 17.6 mg/cig (3.8% ↗) <i>Phosphoric acid extract</i> nicotine: 1.2 mg/cig (0.8% ↗) "tar": 26.5 mg/cig (2.7% ↗) CO: 17.8 mg/cig (2.7% ↗) <i>Citric acid extract</i> nicotine: 1.18 mg/cig (97.5% ↗) "tar": 25.4 mg/cig (1.5% ↗) CO: 18.1 mg/cig (1.1% ↗) <i>Pectin extract + nitric acid</i> nicotine: 1.18 mg/cig (0.8% ↗) "tar": 25.7 mg/cig (2% ↗) CO: 14.8 mg/cig (0.7% ↗) <i>Pectin extract + phosphoric acid</i> nicotine: 1.2 mg/cig (0.8% ↗) "tar": 26.4 mg/cig (4.8% ↗) CO: 15.3 mg/cig (2.7% ↗) <i>Pectin extract + citric acid</i> nicotine: 1.18 mg/cig (0.8% ↗) "tar": 26 mg/cig (3.2% ↗) CO: 14.9 mg/cig (↔)
Phenol	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke TPM: 1.7% ↗ "tar": 2.2% ↗ nicotine: 17.6% ↗ phenol: 2.8% ↗ o-cresol: 7.5% ↗ m-, p-cresol: 5.2% ↗ B[a]P: 89.7% ↗
Phenyl disulfide	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	Bentley and Burgen, 1960 Burton and Benner, 1972
3-Phenyl-5-methyl-1,2,4-oxadiazole (PMO)	2% (w/w) radioactivity: 1.578 µCi/g cig	Tobacco	Mixture with a uniformly cut sample of tobacco with labelled [PMO (5- ¹⁴ C)] and unlabelled PMO → preparation of cigarettes	PMO-recovery: 94.51%	PMO-decomposition to ¹⁴ CO ₂ : 1.48%	Relative percentage of label found (3 runs): TPM: 25.04%; 31.44%; 25.97% butt + ash: 36.72%; 25.84%; 25.86% CO ₂ : 0.57%; 0.73%; 0.86%
						Marmor and Minnemeyer, 1975

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Phenyl-6-methyl-oxadiazole (PMO)	1.5% (w/w) 2.8% (w/w) 5.3% (w/w)	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of cigarettes (SEB IV) + PMO	n.d.	n.d.	Concentration/cigarette TPM: 33.6 mg/cig (7.3% ↗) "tar": 27.2 mg/cig (5.8% ↗) water: 4.59 mg/cig (26.1% ↗) nicotine: 1.84 mg/cig (4.2% ↗) phenol: 166 µg/cig (13.7% ↗) acetaldehyde: 0.948 mg/cig (4.8% ↗) acrolein: 79 µg/cig (27.5% ↗) isoprene: 462 µg/cig (12.8% ↗) HCN: 339 µg/cig (1.5% ↗) formaldehyde: 36 µg/cig (12.5% ↗) NO_x: 537 µg/cig (18.0% ↗) CO: 17.5 mL/cig (8.7% ↗) CO₂: 34.6 mL/cig (4.8% ↗) Concentration/g dry condensate B[a]A: 1.31 µg/g (11.0% ↗) B[a]P: 0.59 µg/g (14.5% ↗) tot. w-acids: 1.63 meq/g (34.5% ↗) fatty acids: 13.30 mg/g (31.4% ↗) OLL-acids: 6.76 mg/g (32.4% ↗) palmitic acid: 4.69 mg/g (36.7% ↗) stearic acid: 1.86 mg/g (38.0% ↗) catechol: 4.38 mg/g (16.3% ↗)
Phenylpropionic acid	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 36.9% ↗ "tar": 37.2% ↗ nicotine: 32.1% ↗ phenol: 45.1% ↗ o-cresol: 52% ↗ m-, p-cresol: 12.3% ↗ B[a]P: 35.9% ↗
Phenyl sulfide	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 25% ↗ "tar": 28% ↗ nicotine: 29% ↗ phenol: 30% ↗ o-cresol: 40% ↗ m-, p-cresol: 19% ↗ B[a]P: 32% ↗
Phosphoric acid	50 mg/cig	Tobacco	n.r.	n.r.	n.r.	smoke-pH: 4.9 (12.5% ↗)

NCI, Report No. 4, 1980

Burton and Benner, 1972

Burton and Benner, 1972

Stedman et al., 1969

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Phytosterols	1–3 × 10 ⁶ dpm/ cig	Cigarette	Impregnation by the n.d. syringe technique with ¹⁴ C-labelled phytosterols (specific activity 0.410 µCi/µm); four major tobacco phytosterols: cholesterol, campesterol, stigmasterol, β-sitosterol	n.d.	Distribution of radioactivity: "tar": 19% volatiles: 1.01% CO ₂ : 0.58% PAH: < 1% butt: 6.7% ash: 1.24%	n.d.	Schmeltz <i>et al.</i> , 1978
Pinene (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Platinum	0.06%	Tobacco blend (cased)	Mixture of tobacco blend with platinum ⇒ simulation of cigarette pyrolysis	n.d.	n.d.	PAH: 6% ↘	Bryant <i>et al.</i> , 1979 (P)
Polyethylene glycols (Carbowax)	10%	Flue-cured tobacco	Impregnation with an aqueous solution	n.d.	n.d.	dry TPM (mg/5 cig): 202 (22.4% ↗)	Blimoria and Nisbet, 1975
Polypropylene glycol	10%	Flue-cured tobacco	Impregnation with an aqueous solution	n.d.	n.d.	dry TPM (mg/5 cig): 217 (31.5% ↗)	Blimoria and Nisbet, 1975
Potassium acetate	1% (w/w)	Reconstituted tobacco sheet	Spraying or dipping	n.d.	n.d.	<i>Reconstituted tobacco</i> with 0.35% NO ₃ -N: NO: 36 µg/puff HCN: 23 µg/puff CO: 2.63 mg/puff <i>Denitrated reconstituted tobacco</i> with 0.06% NO ₃ -N: NO: 16 µg/puff HCN: 46 µg/puff CO: 2.80 mg/puff with 0.05% NO ₃ -N + K-acetate: NO: 9 µg/puff HCN: 21 µg/puff CO: 2.20 mg/puff	Keritsis, 1981 (P)
Potassium acetate	n.r.	Tobacco	Treatment with 2% of aqueous solvent	n.d.	n.d.	"tar": 26.7 mg/cig (2.2% ↘)	Aksu, 1969

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Potassium bromate	4%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Potassium bromide	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Potassium carbonate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: $\pm 0\%$ $\rightarrow$ phenol: 21% $\rightarrow$ o-cresol: 20% $\rightarrow$ m-, p-cresol: 30% $\rightarrow$ B[a]P: $\pm 0\%$ TPM: 38% $\rightarrow$	Burdick <i>et al.</i> , 1969
Potassium carbonate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: $\pm 0\%$ $\rightarrow$ phenol: 21% $\rightarrow$ o-cresol: 20% $\rightarrow$ m-, p-cresol: 30% $\rightarrow$ B[a]P: $\pm 0\%$ TPM: 38% $\rightarrow$	Burton, 1969
Potassium carbonate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 28% $\rightarrow$ "tar": 31% $\rightarrow$ nicotine: 52% $\rightarrow$ phenol: 13% $\rightarrow$ o-cresol: 53% $\rightarrow$ m-, p-cresol: 98% $\rightarrow$ B[a]P: 60% $\rightarrow$	Burton and Benner, 1972
Potassium chlorate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 8% $\rightarrow$ "tar": 5% $\rightarrow$ nicotine: 54% $\rightarrow$ phenol: 40% $\rightarrow$ o-cresol: 20% $\rightarrow$ m-, p-cresol: 19% $\rightarrow$ B[a]P: 41% $\rightarrow$	Burton and Benner, 1972
Potassium chlorate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 60% $\rightarrow$ phenol: 42% $\rightarrow$ o-cresol: 17% $\rightarrow$ m-, p-cresol: 24% $\rightarrow$ B[a]P: 48% $\rightarrow$ TPM: 16% $\rightarrow$	Burdick <i>et al.</i> , 1969
Potassium chlorate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 60% $\rightarrow$ phenol: 42% $\rightarrow$ o-cresol: 17% $\rightarrow$ m-, p-cresol: 24% $\rightarrow$ B[a]P: 48% $\rightarrow$ TPM: 16% $\rightarrow$	Burton, 1969

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Potassium chloride	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Potassium chloride	0–1.0 µg	Powder (0.1 g) of extracted cigarette tobacco	Mixture with leaf powder or powder from extracted cigarettes	n.r.	n.d.	No alkylating activity alteration by KCl	Crosthwaite <i>et al.</i> , 1979
Potassium citrate	2% and 4% (w/w)	Reconstituted tobacco sheet	Spraying or dipping	n.d.	n.d.	Reconstituted tobacco with 0.57% NO ₃ -N: NO: 0.67 mg/cig HCN: 0.17 mg/cig CO: 14 mg/cig Denitrated reconstituted tobacco with 0.05% NO ₃ -N: NO: 0.19 mg/cig HCN: 0.16 mg/cig CO: 15 mg/cig + 2% K-citrate with 0.05% NO ₃ -N: NO: 0.10 mg/cig HCN: 0.09 mg/cig CO: 14 mg/cig + 4% K-citrate with 0.05% NO ₃ -N: NO: 0.08 mg/cig HCN: 0.06 mg/cig CO: 12 mg/cig	Keritsis, 1981 (P)
Potassium iodide	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Potassium lactate	n.r.	Tobacco	Treatment with 2% of aqueous solvent	n.d.	n.d.	"tar": 27.9 mg/cig (2.2% ↗)	Aksu, 1969
Potassium malate	n.r.	Tobacco	Treatment with 2% of aqueous solvent	n.d.	n.d.	"tar": 25.2 mg/cig (7.7% ↘)	Aksu, 1969
Potassium nitrate	N added as nitrate: 1.5%	Tobacco	Spraying of an aqueous solution with labelled ¹⁵ N potassium nitrate	n.r.	acetamide: 30% propionamide: 21% HCN: 45% acetonitrile: 42% acrylonitrile: 38%		Johnson <i>et al.</i> , 1973

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	
Potassium nitrate	2.23% 2.8% 5.3%	Tobacco blend	Addition of KNO ₃ during casing, doubling the total nitrate present ⇒ manufacture of cigarettes	n.d.	n.d.	NCI, Report No.1, 1976
					<i>Concentration/cigarette</i> TPM: 28.66 mg/cig (5.2% ↗) water: 2.94 mg/cig (2.4% ↗) nicotine: 1.65 mg/cig (1.8% ↗) "tar": 24.22 mg/cig (6.5% ↗) acetaldehyde: 1084 µg/cig (1.7% ↗) acrolein: 105.3 µg/cig (3.2% ↗) formaldehyde: 32.23 µg/cig (10.2% ↗) HCN: 164.7 µg/cig (18.1% ↗) NO_x: 774.6 µg/cig (111.2% ↗) CO: 14.49 mL/cig (10% ↗) CO₂: 29.96 mL/cig (3.4% ↗) <i>Concentration/g dry condensate</i> phenol: 3.90 mg/g (10.3% ↗) o-cresol: 0.58 mg/g (25.6% ↗) <i>m</i>-, <i>p</i>-cresol: 1.62 mg/g (11.5% ↗) ColorPheno: 5.81 mg/g (11.3% ↗) tot. w-acids: 2507 meq/g (15.2% ↗) phenanthrene: 16.6 µg/g (28.4% ↗) B[a]A: 0.99 µg/g (17.5% ↗) B[a]P: 0.89 µg/g (23.6% ↗) <i>Concentration in % (w/w) TPM</i> palmitic acids: 0.39 % (15.2% ↗) OLL-acids: 0.63% (13.7% ↗) stearic acids: 0.16% (23.8% ↗) fatty acids: 1.18% (15.7% ↗)	
Potassium nitrate	0.11% 0.34% 0.42% (w/w) in tobacco	Tobacco blend	Flue-cured or burley tobaccos are sprayed with an aqueous solution	n.d.	<i>Control (flue-cured)</i> 0.04% nitrate NO_x: 0.042 mg/cig + 0.34% KNO₃ NO_x: 0.338 mg/cig (704% ↗) + 0.42% KNO₃ NO_x: 0.486 mg/cig (1057% ↗) <i>Control (burley)</i> 0.27% nitrate NO_x: 0.162 mg/cig + 0.11% KNO₃ NO_x: 0.144 mg/cig (11.1% ↗)	Kallianos et al., 1968

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Potassium nitrate [0.11%, 0.34%, 0.42% (w/w), contd.]					+ 0.32% KNO ₃ NO _x : 0.189 mg/cig (16.7% ↗) + 0.79% KNO ₃ NO _x : 0.246 mg/cig (51.9% ↗) n.d.	+ 0.32% KNO ₃ catechol: 56 µg/cig (27.3% ↗) + 0.79% KNO ₃ catechol: 30 µg/cig (61% ↗)
Potassium nitrate	5%	Reconstituted tobacco sheet	Incorporation during the slurry process ⇒ preparation of cigarettes from the treated and non-treated sheets	n.d.	n.d.	Concentration/cigarette TPM: 15.95 mg/cig (13.3% ↗) water: 1.89 mg/cig (4.1% ↗) nicotine: 0.78 mg/cig (12.4% ↗) "tar": 13.28 mg/cig (14.5% ↗) acetaldehyde: 885 µg/cig (7.8% ↗) acrolein: 104.9 µg/cig (0.9% ↗) formaldehyde: 32.1 µg/cig (31.7% ↗) HCN: 143.1 µg/cig (42.1% ↗) NO _x : 403.7 µg/cig (0.6% ↗) CO: 14.43 mL/cig (2.6% ↗) CO ₂ : 21.39 mL/cig (15.6% ↗) Concentration/g dry condensate phenol: 6 mg/g (85.2% ↗) o-cresol: 1.06 mg/g (58.2% ↗) m-, p-cresol: 2.49 mg/g (71.7% ↗) colorim. phenols: 7.99 mg/g (46.9% ↗) tot. w-acids: 2.67 meq/g (1.8% ↗) phenanthrene: 27.3 µg/g (46.0% ↗) B[a]A: 1.44 µg/g (41.2% ↗) B[a]P: 0.98 µg/g (88.5% ↗) Concentration in % (w/w) TPM palmitic acids: 0.25% (3.8% ↗) OLL-acids: 0.39% (11.4% ↗) stearic acids: 0.13% (7.1% ↗) fatty acids: 0.77% (8.3% ↗) Experimental cigarette (cig 22) (compared to cig 20) Concentration/cigarette TPM: 31.35 mg/cig (11.4% ↗) water: 3.52 mg/cig (6.1% ↗) nicotine: 1.42 mg/cig (28.3% ↗) "tar": 26.58 mg/cig (11.5% ↗) acetaldehyde: 1298 µg/cig (11.88% ↗) acrolein: 132.1 µg/cig (53.4% ↗) formaldehyde: 31.1 µg/cig (22.5% ↗) HCN: 119.9 µg/cig (37.1% ↗) NO _x : 421.3 µg/cig (28.0% ↗) CO: 23.31 mL/cig (5.3% ↗) CO ₂ : 29.49 mL/cig (21.4% ↗)
Potassium nitrate	0–1.0 µg	Powder (0.1 g) of extracted cigarette tobacco	Mixture with leaf powder or powder from extracted cigarettes	n.r.	n.d.	Crosthwaite et al., 1979

Table 3 (contd.)

Ingredient	Experimental design		Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Potassium nitrate (0–1.0 µg, contd.)					<i>Concentration/g dry condensate</i> phenol: 2.67 mg/g (37.0% ↗) o-cresol: 0.44 mg/g (29.0% ↗) m-, p-cresol: 1.04 mg/g (45.5% ↗) colorim. phenols: 4.10 mg/g (37.9% ↗) tot. w-acids: 2.07 meq/g (3.7% ↗) phenanthrene: 14.1 µg/g (31.9% ↗) B[a]A: 0.91 µg/g (13.3% ↗) B[a]P: 0.64 µg/g (24.7% ↗) <i>Concentration in % (w/w) TPM</i> palmitic acids: 0.29% (17.1% ↗) OLL-acids: 0.51% (15.0% ↗) stearic acids: 0.15% (0% ↗) fatty acids: 0.95% (13.6% ↗)
Potassium nitrate	2–4% (w/w)	Tobacco	Spraying of an aqueous solution (SEB III)	n.d.	<i>Concentration/cigarette</i> TPM: 31.6 mg/cig (13.7% ↗) "tar": 27.1 mg/cig (12.5% ↗) water: 2.69 mg/cig (28.7% ↗) nicotine: 1.8 mg/cig (10.4% ↗) phenol: 164 µg/cig (3.8% ↗) acetaldehyde: 1.176 mg/cig (5.7% ↗) acrolein: 108 µg/cig (7.7% ↗) isoprene: 460 µg/cig (13.6% ↗) HCN: 338 µg/cig (13.3% ↗) formaldehyde: 34 µg/cig (0.8% ↗) NO_x: 436 µg/cig (1.0% ↗) CO: 16.1 mL/cig (0.5% ↗) CO₂: 32.6 mL/cig (4.9% ↗) <i>Concentration/g dry condensate</i> indole: 463 µg/g (36.4% ↗) skatole: 315 µg/g (8.3% ↗) B[a]A: 1.41 µg/g (16.5% ↗) B[a]P: 1.02 µg/g (2.0% ↗) o-cresol: 0.70 mg/g (2.9% ↗) m-, p-cresol: 1.93 mg/g (2.5% ↗) tot. w-acids: 2.24 meq/g (6.7% ↗) fatty acids: 21.61 mg/g (7.1% ↗) OLL-acids: 12.92 mg/g (6.5% ↗) palmitic acid: 6.60 mg/g (5.2% ↗) stearic acid: 2.09 mg/g (15.4% ↗) catechol: 5.18 mg/g (12.8% ↗) glycerol: 78.03 mg/g
					Bentley and Burgan, 1960

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Potassium nitrate	5% (w/w)	Cigarette ("bright yellow" or "Matsukawa" tobacco) SEB III	n.r.	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 33.39 mg/cig (20.1% ↗) "tar": 27.99 mg/cig (16.2% ↗) water: 3.77 mg/cig (80.4% ↗) nicotine: 1.63 mg/cig (0% →) phenol: 199.92 µg/cig (26.6% ↗) acetaldehyde: 1.32 mg/cig (18.7% ↗) acrolein: 133.38 µg/cig (33.0% ↗) isoprene: 546.25 µg/cig (2.6% ↗) HCN: 510.5 µg/cig (71.2% ↗) formaldehyde: 34.5 µg/cig (2.3% ↗) NO_x: 1379 µg/cig (213.1% ↗) CO: 17.65 mL/cig (916% ↗) CO₂: 38.25 mL/cig (23.1% ↗) <i>Concentration/g dry condensate</i> indole: 439.8 µg/g (39.6% ↗) skatole: 303.2 µg/g (11.7% ↗) B[a]A: 1.43 µg/g (18.2% ↗) B[a]P: 1.21 µg/g (21.0% ↗) o-cresol: 0.52 mg/g (23.5% ↗) m-, p-cresol: 1.61 mg/g (18.7% ↗) colorim. phenols: 5.36 mg/g (24.7% ↗) tot. w-acids: 2.12 meq/g (11.7% ↗) fatty acids: 21.25 mg/g (8.6% ↗) OLL-acids: 12.83 mg/g (7.2% ↗) palmitic acid: 6.23 mg/g (10.5% ↗) stearic acid: 2.10 mg/g (15.0% ↗) neophytadiene: 9.64 mg/g (3.5% ↗) catechol: 4.74 mg/g (20.2% ↗) glycerol: 72.2 mg/g	Kaburaki et al., 1969
Potassium nitrate	2%	Cigarette (SEB III)	n.r.	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 26.34 mg/cig (5.3% ↗) "tar": 22.37 mg/cig (7.1% ↗) water: 2.47 mg/cig (18.2% ↗) nicotine: 1.49 mg/cig (8.6% ↗) phenol: 169.92 µg/cig (7.6% ↗) acetaldehyde: 1.12 mg/cig (0.7% ↗) acrolein: 100.38 µg/cig (0.1% ↗) isoprene: 542.5 µg/cig (1.9% ↗) HCN: 59 µg/cig (80.2% ↗) formaldehyde: 37.6 µg/cig (11.5% ↗) NO_x: 406.41 µg/cig (7.7% ↗) CO: 14.89 mL/cig (8.0% ↗) CO₂: 32.86 mL/cig (5.8% ↗)	Garcia Roche et al., 1986 (A)

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Potassium nitrate (2%, contd.)						<i>Concentration/g dry condensate</i> indole: 716.3 µg/g (1.6% ↗) skatole: 381.7 µg/g (11.2% ↗) B[a]A: 1.56 µg/g (28.9% ↗) B[a]P: 1.38 µg/g (38.0% ↗) o-cresol: 0.69 mg/g (1.5% ↗) <i>m</i>-, <i>p</i>-cresol: 1.92 mg/g (3.0% ↗) colorim. phenols: 6.71 mg/g (5.8% ↗) tot. w-acids: 1.92 meq/g (20.0% ↗) fatty acids: 19.28 mg/g (17.1% ↗) OLL-acids: 11.23 mg/g (18.7% ↗) palmitic acid: 5.96 mg/g (14.4% ↗) stearic acid: 2.09 mg/g (15.4% ↗) neophytadiene: 9.98 mg/g (0.1% ↗) catechol: 4.25 mg/g (18.5% ↗) glycerol: 92.0 mg/g
Potassium nitrate	4%	Tobacco (SEB III)	n.r.	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 25.57 mg/cig (8.0% ↗) "tar": 22.34 mg/cig (7.3% ↗) water: 2.08 mg/cig (0.5% ↗) nicotine: 1.14 mg/cig (30.1% ↗) phenol: 102.0 µg/cig (35.4% ↗) acetaldehyde: 1.238 mg/cig (11.3% ↗) acrolein: 131.38 µg/cig (31.1% ↗) isoprene: 457.5 µg/cig (14.1% ↗) HCN: 93.38 µg/cig (68.7% ↗) formaldehyde: 39.47 µg/cig (17.1% ↗) NO_x: 1407 µg/cig (219.6% ↗) CO: 14.27 mL/cig (11.8% ↗) CO₂: 32.5 mL/cig (4.6% ↗) <i>Concentration/g dry condensate</i> indole: 545.1 µg/g (25.2% ↗) skatole: 360.4 µg/g (5.0% ↗) B[a]A: 1.44 µg/g (19.0% ↗) B[a]P: 1.17 µg/g (17.0% ↗) o-cresol: 0.53 mg/g (22.1% ↗) <i>m</i>-, <i>p</i>-cresol: 1.58 mg/g (20.2% ↗) colorim. phenols: 6.04 mg/g (15.2% ↗) tot. w-acids: 1.72 meq/g (28.3% ↗) fatty acids: 19.34 mg/g (16.8% ↗) OLL-acids: 10.94 mg/g (20.8% ↗) palmitic acid: 5.86 mg/g (15.8% ↗) stearic acid: 2.03 mg/g (17.8% ↗) neophytadiene: 10.52 mg/g (5.3% ↗) catechol: 3.6 mg/g (39.4% ↗) glycerol: 70.9 mg/g
						Pyriki et al., 1965

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Potassium nitrate	2.46 and 5.05%	Cut tobacco (SEB III)	Spraying with a 50% KNO ₃ solution	n.d.	n.d.	Concentration/cigarette TPM: 25.57 mg/cig (19.1% ↗) "tar": 22.34 mg/cig (17.6% ↗) water: 2.08 mg/cig (22.7% ↗) nicotine: 1.14 mg/cig (36.7% ↗) phenol: 102.0 µg/cig (37.8% ↗) acetaldehyde: 1.238 mg/cig (5.3% ↗) acrolein: 131.38 µg/cig (21.6% ↗) isoprene: 457.5 µg/cig (0.5% ↗) HCN: 93.38 µg/cig (35.4% ↗) formaldehyde: 39.47 µg/cig (16.1% ↗) NO_x: 1407 µg/cig (222.7% ↗) CO: 14.27 mL/cig (11.4% ↗) CO₂: 32.5 mL/cig (0.3% ↗) Concentration/g dry condensate indole: 545.1 µg/g (17.7% ↗) skatole: 360.4 µg/g (14.4% ↗) B[a]A: 1.44 µg/g (2.1% ↗) B[a]P: 1.17 µg/g (14.7% ↗) o-cresol: 0.53 mg/g (24.3% ↗) m-, p-cresol: 1.58 mg/g (18.1% ↗) tot. w-acids: 1.72 meq/g (23.2% ↗) fatty acids: 19.34 mg/g (10.5% ↗) OLL-acids: 10.94 mg/g (15.3% ↗) palmitic acid: 5.86 mg/g (11.2% ↗) stearic acid: 2.03 mg/g (2.9% ↗) catechol: 3.6 mg/g (30.5% ↗) glycerol: 70.9 mg/g (9.1% ↗)	Rathkamp and Hoffmann, 1970
Potassium nitrate	6.96 and 8.07%	Cut tobacco	Spraying with a 50% KNO ₃ solution	n.d.	n.d.	Concentration/cigarette TPM: 24.5 mg/cig (27.9% ↗) "tar": 20.3 mg/cig (29.5% ↗) water: 3.24 mg/cig (5.0% ↗) nicotine: 0.96 mg/cig (44.5% ↗) phenol: 48 µg/cig (60.3% ↗) acetaldehyde: 666 µg/cig (33.2% ↗) acrolein: 98 µg/cig (10.1% ↗) isoprene: 374 µg/cig (4.6% ↗) HCN: 344 µg/cig (8.0% ↗) formaldehyde: 34 µg/cig (15.0% ↗) NO_x: 430 µg/cig (25.7% ↗) CO: 19.6 mL/cig (24.3% ↗) CO₂: 28.8 mL/cig (29.2% ↗)	Rathkamp and Hoffmann, 1970

Table 3 (contd.)

Ingredient	Experimental design		Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Potassium nitrate (6.96 and 8.07%, contd.)					<i>Concentration/g dry condensate</i> indole: 187 mg/g (56.1% ↗) skatole: 334 mg/g (3.5% ↗) B[a]A: 1.17 µg/g (9.3% ↗) B[a]P: 0.81 µg/g (1.3% ↗) o-cresol: 0.57 mg/g (39.0% ↗) m-, p-cresol: 1.19 mg/g (26.5% ↗) colorim. phenols: 4.62 mg/g (12.3% ↗) tot. w-acids: 3.30 meq/g (35.2% ↗) fatty acids: 16.28 mg/g (14.3% ↗) OLL-acids: 8.71 mg/g (11.9% ↗) palmitic acid: 5.03 mg/g (18.3% ↗) stearic acid: 2.54 mg/g (17.0% ↗) neophytadiene: 5.67 mg/g (32.9% ↗) glycerol: 85.2 mg/g (16.5% ↗) catechol: 4.72 mg/g (8.3% ↗)
Potassium sorbate	40 µg/g tobacco	Tobacco	Impregnation of tobacco with a potassium sorbate solution	filter cigarette: 12.9–14.4% sorbate plain cigarette: 21.4% sorbate	<i>Concentration/cigarette</i> TPM: 26.7 mg/cig (21.5% ↗) "tar": 23.1 mg/cig (19.8% ↗) water: 3.21 mg/cig (5.9% ↗) nicotine: 0.36 mg/cig (79.2% ↗) phenol: 109 µg/cig (9.1% ↗) acetaldehyde: 803 µg/cig (19.5% ↗) acrolein: 93 µg/cig (14.7% ↗) isoprene: 321 µg/cig (18.1% ↗) HCN: 248 µg/cig (33.7% ↗) formaldehyde: 58 µg/cig (45.0% ↗) NO_x: 349 µg/cig (39.7% ↗) CO: 22.0 mL/cig (15.1% ↗) CO₂: 31.3 mL/cig (23.1% ↗) <i>Concentration/g dry condensate</i> indole: 260 mg/g (39.0% ↗) skatole: 438 mg/g (26.6% ↗) B[a]A: 0.83 µg/g (22.4% ↗) B[a]P: 0.69 µg/g (13.7% ↗) o-cresol: 0.58 mg/g (41.5% ↗) m-, p-cresol: 1.52 mg/g (6.2% ↗) colorim. phenols: 6.5 mg/g (23.3% ↗) tot. w-acids: 2.38 meq/g (2.5% ↗) fatty acids: 15.91 mg/g (16.2% ↗) OLL-acids: 7.75 mg/g (20.8% ↗) palmitic acid: 5.21 mg/g (15.4% ↗) stearic acid: 2.95 mg/g (3.6% ↗) neophytadiene: 5.27 mg/g (37.6% ↗) glycerol: 77.6 mg/g (23.9% ↗) catechol: 5.42 mg/g (5.2% ↗)

Brunnemann and
Posset, 1980

n.d.

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Proline	5% (w/w)	Cigarette ("bright yellow" or "Matsukawa" tobacco)	n.r.	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 17.9 mg/cig (28.7% ↗) "tar": 13.3 mg/cig (32.8% ↗) water: 3.53 mg/cig (16.0% ↗) nicotine: 1.06 mg/cig (10.2% ↗) phenol: 52 µg/cig (21.2% ↗) acetaldehyde: 480 µg/cig (43.4% ↗) acrolein: 65 µg/cig (46.3% ↗) isoprene: 82 µg/cig (69.5% ↗) HCN: 2158 µg/cig (13.7% ↗) formaldehyde: 17 µg/cig (46.9% ↗) NO_x: 314 µg/cig (44.7% ↗) CO: 12.2 mL/cig (29.5% ↗) CO₂: 26.6 mL/cig (1.5% ↗) <i>Concentration/g dry condensate</i> indole: 170 mg/g (20.6% ↗) skatole: 208 mg/g (24.1% ↗) B[a]A: 1.60 µg/g (122.2% ↗) B[a]P: 1.11 µg/g (91.4% ↗) o-cresol: 0.67 mg/g (24.1% ↗) m-, p-cresol: 1.33 mg/g (8.9% ↗) colorim. phenols: 4.8 mg/g (19.1% ↗) tot. w-acids: 2.00 meq/g (34.4% ↗) fatty acids: 12.33 mg/g (14.5% ↗) OLL-acids: 5.32 mg/g (8.1% ↗) palmitic acid: 4.23 mg/g (32.2% ↗) stearic acid: 2.79 mg/g (57.6% ↗) neophytadiene: 2.25 mg/g (51.9% ↗) glycerol: 151 mg/g (31.3% ↗) catechol: 5.41 mg/g (1.3% ↗) <i>Concentration/cigarette</i> TPM: 2.5 mg/cig (92.6% ↗) "tar": 1.9 mg/cig (93.4% ↗) water: 0.51 mg/cig (85.0% ↗) nicotine: 0.09 mg/cig (94.8% ↗) phenol: 34 µg/cig (71.9% ↗) acetaldehyde: 304 µg/cig (69.5% ↗) acrolein: 71 µg/cig (34.9% ↗) isoprene: 76 µg/cig (80.6% ↗) HCN: 0 µg/cig (100.0% ↗) formaldehyde: 10 µg/cig (75.0% ↗) NO_x: 174 µg/cig (69.9% ↗) CO: 4.4 mL/cig (83.0% ↗) CO₂: 19.9 mL/cig (51.1% ↗)	Kaburaki et al., 1969
Propylene glycol	n.r.	n.r.	n.r.	Sample A: 0.38–0.44 mg/cig Sample B: 0.95–1.03 mg/cig	n.d.		Lyerly, 1967

Table 3 (contd.)

Ingredient	Experimental design		Results		Reference(s)
	Amount	Application to application	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Propylene glycol (n.r., contd.)					<i>Concentration/g dry condensate</i> indole: 8.2 mg/g (98.1% ↗) skatole: 56 mg/g (83.8% ↗) B[a]A: 3.34 µg/g (212.1% ↗) B[a]P: 1.78 µg/g (122.5% ↗) o-cresol: 0.17 mg/g (58.5% ↗) m-, p-cresol: 0.43 mg/g (73.5% ↗) colorim. phenols: 1.45 mg/g (72.5% ↗) tot. w-acids: 2.20 meq/g (9.8% ↗) fatty acids: 17.19 mg/g (9.5% ↗) OLL-acids: 7.65 mg/g (21.8% ↗) palmitic acid: 5.67 mg/g (8.0% ↗) stearic acid: 3.87 mg/g (26.5% ↗) neophytadiene: 3.17 mg/g (62.5% ↗) glycerol: 170 mg/g (66.7% ↗) catechol: 3.15 mg/g (38.8% ↗)
Propylene glycol	0.38% on tobacco	Filter cigarette	n.r.	70 mm test cigarette 0.86 mg/g tobacco ⇒ 19.2% transfer	Experimental cigarette (cig 5) (compared to cig 2)
	0.6–0.7% on tobacco			85 mm filter cigarette 0.36–0.46 mg/g tobacco ⇒ 4.1–4.9% transfer	<i>Concentration/cigarette</i> TPM: 28.66 mg/cig (5.2% ↗) water: 2.94 mg/cig (2.4% ↗) nicotine: 1.65 mg/cig (1.8% ↗) "tar": 24.22 mg/cig (6.5% ↗) acetaldehyde: 1084 µg/cig (1.7% ↗) acrolein: 105.3 µg/cig (3.2% ↗) formaldehyde: 32.23 µg/cig (10.2% ↗) HCN: 164.7 µg/cig (18.1% ↗) NO_x: 774.6 µg/cig (111.2% ↗) CO: 14.49 mL/cig (10% ↗) CO₂: 29.96 mL/cig (3.4% ↗) <i>Concentration/g dry condensate</i> phenol: 3.90 mg/g (10.3% ↗) o-cresol: 0.58 mg/g (25.6% ↗) m-, p-cresol: 1.62 mg/g (11.5% ↗) colorim. phenols: 5.81 mg/g (11.3% ↗) tot. w-acids: 2507 meq/g (15.2% ↗) phenanthrene: 16.6 µg/g (28.4% ↗) B[a]A: 0.99 µg/g (17.5% ↗) B[a]P: 0.89 µg/g (23.6% ↗) <i>Concentration in % (w/w) TPM</i> palmitic acids: 0.39% (15.2% ↗) OLL-acids: 0.63% (13.7% ↗) stearic acids: 0.16% (23.8% ↗) fatty acids: 1.18% (15.7% ↗)
				n.d.	Laurene et al., 1965

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Propylene glycol	n.r.	Cigarette	n.r.	Transfer rates for propylene glycol were more affected by filter ventilation than were those for glycerol	n.r.	n.r.	Cook <i>et al.</i> , 1999 (A)
Propylene glycol	2.8–9.4 mg/g tobacco	Cigarette	n.r.	n.r.	propylene oxide: 370 ng/g tobacco	n.d.	Kagan <i>et al.</i> , 1999 (A)
Propylene glycol	10%	Flue-cured tobacco	Impregnation with an aqueous solution	n.d.	n.d.	dry TPM (mg/5 cig): 124 (24.8% ↘)	Bilimoria and Nisbet, 1975
Propylene glycol	2 and 3%	Tobacco	Diluted with water by spraying ⇒ manufacture of cigarettes	n.d.	n.d.	2%: nicotine: 1.17 mg/cig (1.7% ↘) "tar": 26.8 mg/cig (6.3% ↘) CO: 15.3 mg/cig (2.7% ↘) 3%: nicotine: 1.18 mg/cig (0.8% ↘) "tar": 27.1 mg/cig (7.5% ↘) CO: 15.7 mg/cig (5.4% ↘) nicotine: 2.33–3.06 mg/cig (2.9–4.4% ↘) TPM: 43.5 mg/cig (3.5% ↘) dry condensate: 40.5 mg/cig (3.6% ↘)	Stoilova <i>et al.</i> , 1994
1,2-Propylene glycol	3%	Tobacco	Addition to dried tobacco	n.d.	n.d.	nicotine: 2.33–3.06 mg/cig (2.9–4.4% ↘) TPM: 43.5 mg/cig (3.5% ↘) dry condensate: 40.5 mg/cig (3.6% ↘)	Smit, 1970
Propylene glycol	3.42% (43.8 mg/cig)	Cigarette	Addition during casing of cigarette tobacco	plain cigarette: 3.16 mg/cig ⇒ transfer rate 12.6% filter cigarette: 3.09 mg/cig ⇒ transfer rate 9.9%	n.d.	polyol: 7.78 mg/cig (6.6% ↘) nicotine: 5.11 mg/cig (14.3% ↘) volatile acids: 2.27 mg/cig (21.2% ↘) 2,4-DNP: 7.67 mg/cig (7% ↘) acetaldehyde: 0.92 mg/cig (13.6% ↘) propionaldehyde: 0.05 mg/cig (25% ↘) acetone: 0.14 mg/cig (75% ↘)	Kobashi <i>et al.</i> , 1965
Pyridine (in α-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Pyridine (in tri- <i>o</i> -thymoid)	1%	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969(P)
Pyromellitic acid	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 11% ↗ "tar": 11% ↗ nicotine: 2% ↗ phenol: 29% ↗ <i>o</i> -cresol: 40% ↗ <i>m</i> -, <i>p</i> -cresol: 32% ↗ B[a]P: 40% ↗	Burton and Benner, 1972
Rutin	0, 2, 4 and 7 mg/cig	Tobacco	Spraying with 3.4 mL MeOH containing varying amounts of rutin ⇒ preparation of cigarettes	n.d.	Contribution of rutin to MSS catechol: <1%	n.d.	Carmella <i>et al.</i> , 1984

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Silver nitrate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
β -Sitosterol	n.r.	Cigarette	Syringe injection of a chloroform solution of β -sitosterol-4- 14 C	Average transfer of 14 C-labelled β -sitosterol: 16.20% butt: 3.09% ash: 0.007%	n.d.	n.d.	Cheng, 1973
Sodium antimonate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 48.3% ↗ "tar": 50% ↗ nicotine: 21.4% ↗ phenol: 19.7% ↗ o-cresol: 16% ↗ m-, p-cresol: 5.5% ↗ B[a]P: 10.3% ↗	Burton and Benner, 1972
Sodium borate	0.8%	Cigarette paper	Impregnation with an aqueous solution	n.d.	n.d.	CO: 6.7% ↗ "tar": 14.6% ↗ nicotine: 7.1% ↗	Baldry <i>et al.</i> , 1988
Sodium citrate	2.5%	Cigarette paper	Impregnation with an aqueous solution	n.d.	n.d.	CO: 17.9% ↗ "tar": 6.4% ↗ nicotine: 3.6 ↗	Baldry <i>et al.</i> , 1988
Sodium dichromate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 6% ↗ "tar": 4% ↗ nicotine: 28% ↗ phenol: 44% ↗ o-cresol: 83% ↗ m-, p-cresol: 88% ↗ B[a]P: 349% ↗	Burton and Benner, 1972
Sodium fluoride	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 1% ↗ "tar": 3% ↗ nicotine: 32% ↗ phenol: 6% ↗ o-cresol: 36% ↗ m-, p-cresol: 42% ↗ B[a]P: 40% ↗	Burton and Benner, 1972
Sodium hydrogen carbonate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 16% ↗ "tar": 17% ↗ nicotine: 33% ↗ phenol: 13% ↗ o-cresol: 43% ↗ m-, p-cresol: 85% ↗ B[a]P: 13% ↗	Burton and Benner, 1972
Sodium iodate	5%	Tobacco 1R1-cigarette	Spraying of an aqueous solution	n.d.	n.d.	TPM: 1.1% ↗ "tar": 1.9% ↗ nicotine: 10.7% ↗ phenol: 35.9% ↗ o-cresol: 96% ↗ m-, p-cresol: 37% ↗ B[a]P: 94.9% ↗	Burton and Benner, 1972

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Sodium iodate (5%, contd.)		Tobacco SB-cigarette				TPM: 19.8% ↗ "tar": 25.4% ↗ nicotine: 44.1% ↗ phenol: 9% ↗ o-cresol: 25% ↗ m-, p-cresol: 13% ↗ B[a]P: 110.3% ↗	Burton and Benner, 1972
Sodium malate	2.5% (w/w)	Cigarette paper	Impregnation with an aqueous solution	n.d.	n.d.	CO: 37.1% ↗ "tar": 3.2% ↗ nicotine: ± 0%	Baldry <i>et al.</i> , 1988
Sodium molybdate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 17% ↗ "tar": 15% ↗ nicotine: 30% ↗ phenol: 79% ↗ o-cresol: 103% ↗ m-, p-cresol: 67% ↗ B[a]P: 36% ↗	Burton and Benner, 1972
Sodium nitrate	8%	Cigarette	n.r.	n.d.	n.d.	TPM: 27 mg/cig (6.9% ↗) nicotine: 1.4 mg/cig (22.2% ↗) NDMA: 95 ng/cig (± 95 ng)	Morie and Sloan, 1973
Sodium nitrate	8.3%	Tobacco blend	In powdered form, added by dusting	n.d.	n.d.	DPM: 19 mg/cig (31.6% ↗) nicotine: 0.91 mg/cig (51.6% ↗) phenol: 60.4 µg/cig (37.1% ↗) B[a]P: 9.5 ng/cig (68.2% ↗)	Hoffmann and Wynder, 1967
Sodium nitrate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 63% ↗ phenol: 35% ↗ o-cresol: 40% ↗ m-, p-cresol: 65% ↗ B[a]P: 34% ↗ TPM: 63% ↗	Burdick <i>et al.</i> , 1969
Sodium nitrate	8%	Cigarette tobacco	n.r.	n.d.	n.d.	DPM: 22.9 mg/cig (68.8% ↗) nicotine: 1.03 mg/cig (43.1% ↗) phenol: 0.136 mg/cig (25.7% ↗) CO: 12.1 mL/cig (11% ↗) NO: 3530 ppm (579% ↗) B[a]P: 0.75 ppm (28.6% ↗) acrolein: 71 µg/cig (16.4% ↗) acetaldehyde: 1.66 mg/cig (16.9% ↗) HCN: 0.29 µg/cig (3.6% ↗)	Dontenwill <i>et al.</i> , 1972
Sodium nitrate	Nitrate added as N: 1.8%	Tobacco	Spraying of an aqueous solution with labelled ¹⁵ N sodium nitrate	n.r.	HCN: 58% acetonitrile: 56% acrylonitrile: 50%	n.d.	Johnson <i>et al.</i> , 1973
Sodium nitrate	1.8%	Tobacco	n.r.	n.d.	n.d.	DPM: 28.7 mg/cig (6.5% ↗) nicotine: 1.5 mg/cig (11.2% ↗) phenol: 0.169 mg/cig (5.1% ↗) B[a]P in "tar": 1.36 ppm (2.2% ↗)	Dontenwill <i>et al.</i> , 1976

Table 3 (contd.)

Ingredient	Experimental design		Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS
Sodium nitrate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 36.7% ↗ "tar": 34.6% ↗ nicotine: 64.7% ↗ phenol: 14.7% ↗ o-cresol: 12.5% ↗ m-, p-cresol: 43.5% ↗ B[a]P: 43.9% ↗
Sodium nitrate	6.6 or 8% NaNO ₃	Reconstituted tobacco sheets and cigarettes	Incorporation into cigarettes or tobacco sheet by impregnation	n.d.	n.d.	Cigarette + 8% NaNO ₃ 3 different condensate fractions TPM2: 73.2 g/100 g (1.3% ↗) TPM4: 18.1 g/100 g (11.7% ↗) TPM5: 5.4 g/100 g (2.5% ↗) aliph. hydrocarb.: 6.1% (11.7% ↗) nicotine (fraction 5): 0.42% (91.6% ↗) phenol (fraction 5): 0.31% (27.9% ↗) Sheet + 6.6% NaNO ₃ 3 different condensate fractions TPM2: 81.0 g/100 g (2.5% ↗) TPM4: 13.3 g/100 g (4.7% ↗) TPM5: 3.7 g/100 g (19.6% ↗) aliph. hydrocarb.: 1.0% (9.1% ↗) nicotine (fraction 5): 0.21% (94.5% ↗) phenol (fraction 5): 0.09% (43.7% ↗)
Sodium nitrate	0.52, 1.2, 1.8, 2.4 and 3.05%	Tobacco	Syringe injection: solutions 5.38–21.5 mg sodium nitrate/0.05 mL	n.d.	n.d.	Control (0.52% sodium nitrate): "tar": 32.2 mg/cig nicotine: 3.2 mg/cig CO: 18.3 mg/cig CO ₂ : 64.6 mg/cig catechol: 167 µg/cig B[a]P: 26 ng/cig NO: 235 µg/cig NDMA: 17 ng/cig NPYR: 38 ng/cig NNN: 239 ng/cig NNK: 108 ng/cig NAT/NAB: 256 ng/cig 1.2–3.05% sodium nitrate: "tar": 5–13% ↗ nicotine: 6–21.9% ↗ B[a]P: 15.4–23.1% ↗ at higher concentrations (2.4 and 3.05%) catechol: 20.4–41.3% ↗ NO: 55.3–166% ↗ NDMA: 76.5–282.4% ↗ NPYR: 97.4–505% ↗ NNN: 13–55.2% ↗ NNK: 0–34.3% ↗ NAT/NAB: 28.1–306.5 ↗ no significant alteration of CO/CO ₂

Burton and
Benner, 1972

Klimisch, 1972

Adams et al.,
1984

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Sodium nitrate	5.8%	Cigarette	n.r.	n.d.	n.d.	NO: 206.8 (5006% ↗) NO ₂ : 13.75 (4483% ↗) <i>Fifth puff (35 mL)</i> H ₂ : 1.64 mol% (18.8% ↗) O ₂ : 12.46 mol% (7.4% ↘) CO: 3.55 mol% (18.3% ↗) CO ₂ : 7.86 mol% (5.8% ↗) NO + NO ₂ : 48.7 µg (113% ↗) N ₂ O: 11 µg (> 1100% ↗) HCN: 23.3 µg (1.3% ↗) H ₂ S: 0.3 µg (93.3% ↘) CH ₄ : 90 µg (16.3% ↘) C ₂ H ₆ : 36.4 µg (3.7% ↘) acetaldehyde: 146.3 µg (97.7% ↗) acetone: 55.3 µg (36.2% ↗) acetonitrile: 29.3 µg (104.9% ↗) acrolein: 18.4 µg (100% ↗) formaldehyde: 5.6 µg (5.7% ↗)	Sloan and Kiefer, 1969 Terrell and Schmeltz, 1968
Sodium nitrate	8.3%	Cigarette	n.r.	n.d.	n.d.	<i>Fifth puff (35 mL)</i> H ₂ : 1.64 mol% (100% ↗) O ₂ : 12.46 mol% (11.1% ↘) CO: 3.55 mol% (99.4% ↗) CO ₂ : 7.86 mol% (44% ↗) NO + NO ₂ : 48.7 µg (220% ↗) N ₂ O: 11 µg (↗ > 10 µg) HCN: 23.3 µg (76.5% ↗) H ₂ S: 0.3 µg (80% ↘) SO ₂ : 2.7 µg (42.1% ↗) CH ₄ : 90 µg (28.8% ↗) C ₂ H ₆ : 36.4 µg (59% ↗) ethylene: 21.5 µg (100.9% ↗) acetaldehyde: 146.3 µg (211.9% ↗) acetone: 55.3 µg (104.8% ↗) acetonitrile: 29.0 µg (126.5% ↗) acrolein: 18.4 µg (122.8% ↗) formaldehyde: 5.6 µg (14.3% ↗) methanol + methyl chloride + methyl acetylene: 55.2 µg (129% ↗)	Terrell and Schmeltz, 1970
Sodium nitrate	8.3%	Tobacco	Additiv powder mixed with humidified tobacco in a sealed plastic bag	n.d.	n.d.		
Sodium nitrate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 63% ↗ phenol: 35% ↗ o-cresol: 40% ↗ m-, p-cresol: 65% ↗ B[a]P: 34% ↗ TPM: 63% ↗	Burton, 1969
Sodium nitrate	8.3%	Tobacco	Manufacture of treated and untreated cigarettes	n.d.	n.d.	B[a]P: 9.5 µg/cig (67.2% ↘) phenol: 60 µg/cig (37.5% ↘)	Wynder and Hoffmann, 1969

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Sodium nitrite	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 57% ↗ phenol: 40% ↗ o-cresol: 56% ↗ m-, p-cresol: 62% ↗ B[a]P: 47% ↗ TPM: 64% ↗	Burdick <i>et al.</i> , 1969
Sodium nitrite	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 37.5% ↗ "tar": 35.7% ↗ nicotine: 58.8% ↗ phenol: 27.5% ↗ o-cresol: 12.5% ↗ m-, p-cresol: 35.7% ↗ B[a]P: 32.7% ↗	Burton and Benner, 1972
Sodium nitrite	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	B[a]P (content in smoke of 500 g tobacco): 1.7 µg (73% ↗)	Bentley and Burgan, 1960
Sodium nitrite	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 57% ↗ phenol: 40% ↗ o-cresol: 56% ↗ m-, p-cresol: 62% ↗ B[a]P: 47% ↗ TPM (dry): 64% ↗	Burton, 1969
Sodium periodate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 6.9% ↗ "tar": 8.9% ↗ nicotine: 20.6% ↗ phenol: 13.3% ↗ o-cresol: 42.5% ↗ m-, p-cresol: 14.8% ↗ B[a]P: 325.2% ↗	Burton and Benner, 1972
Sodium permanganate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 27.7% ↗ "tar": 29.5% ↗ nicotine: ± 0% phenol: 0.7% ↗ o-cresol: 16% ↗ m-, p-cresol: 8.2% ↗ B[a]P: 10.3% ↗	Burton and Benner, 1972
Sodium stannate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 23.8% ↗ "tar": 25.3% ↗ nicotine: ± 0% phenol: 1.4% ↗ o-cresol: 36% ↗ m-, p-cresol: 2.7% ↗ B[a]P: 20.5% ↗	Burton and Benner, 1972
Sodium tetraborate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	
Sodium thiocyanate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 34% ↗ "tar": 33.5% ↗ nicotine: 41.2% ↗ phenol: 48.8% ↗ o-cresol: 72.5% ↗ m-, p-cresol: 74.8% ↗ B[a]P: 73.8% ↗
Sodium thiosulfate	70 mg/cig	Cigarette	Syringe injection	n.d.	n.d.	TPM: 25.2 mg/cig (10% ↗) B[a]P: 0.096 µg/cig (43.3% ↗) nicotine: 1.31 mg/cig (33.5% ↗) phenol: 299 µg/cig (35.9% ↗)
Sodium vanadate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 54% ↗ phenol: 30% ↗ o-cresol: 30% ↗ m-, p-cresol: 20% ↗ B[a]P: 50% ↗ TPM: 6% ↗
Sodium vanadate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 62% ↗ phenol: 110% ↗ o-cresol: 190% ↗ m-, p-cresol: 110% ↗ B[a]P: 50% ↗ TPM: 31% ↗
Sodium vanadate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 31.9% ↗ "tar": 31.5% ↗ nicotine: 41.2% ↗ phenol: 93.8% ↗ o-cresol: 97.5% ↗ m-, p-cresol: 127% ↗ B[a]P: 28% ↗
Sodium vanadate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 54% ↗ phenol: 30% ↗ o-cresol: 30% ↗ m-, p-cresol: 20% ↗ B[a]P: 50% ↗ TPM: 6% ↗
Sodium vanadate	10%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	nicotine: 42% ↗ phenol: 110% ↗ o-cresol: 190% ↗ m-, p-cresol: 110% ↗ B[a]P: 50% ↗ TPM: 31% ↗
Sorbitol	3%	Tobacco	Addition to dried tobacco	n.d.	n.d.	nicotine: 2.42–3.15 mg/cig (0–0.7% ↗) TPM: 45.5 mg/cig (0.9% ↗) dry condensate: 41.2 mg/cig (1.9% ↗)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Sorbitol	3%	Tobacco	n.r.	n.d.	n.d.	B[a]P: 1.3 µg/100 cig (62.5% ↗) "tar": 29.0 mg/cig (6.2% ↗)	Pyriki <i>et al.</i> , 1965 Aksu, 1969
Sorbitol	n.r.	Tobacco	Treatment with 2% aqueous solution	n.d.	n.d.		
Starch	0–8%	Powder (0.1 g) of extracted cigarette tobacco	Mixture with leaf powder or powder from extracted cigarettes	n.r.	n.d.	No alkylating activity alteration by starch	Crosthwaite <i>et al.</i> , 1979
Stearic acid	1–3 × 10 ⁶ dpm/cig	Cigarette	Impregnation by the n.d. syringe technique with ¹⁴ C-labelled stearic acid (specific activity 0.088 µCi/µm)	n.d.	Distribution of radioactivity (as fatty acids: 95% palmitic acid): "tar": 22.81% volatiles: 0.9% CO ₂ : 1.41% butt: 3.5% ash: 0.6%		Schmeltz <i>et al.</i> , 1978
Sucrose	7 µCi of sucrose- ¹⁴ C/cig	Burley tobacco	Spraying of an alcoholic solution of ¹⁴ C-sucrose (15 mCi/mol)	~ 0.5% of sucrose	Gas phase (percentage of total activity): CO ₂ : 3.1% CO: 2.4% organic comp.: 0.4% TPM: 8.2%	n.d.	Gager <i>et al.</i> , 1971a
Sucrose	7 µCi of sucrose- ¹⁴ C/cig	Burley tobacco	Spraying of an alcoholic solution of ¹⁴ C-sucrose (15 mCi/mol)	n.r.	% of ¹⁴ C in glucose: acetaldehyde: 0.06 furan: 0.01 propionaldehyd: <0.01 acetone: 0.1 acrolein: <0.01 2-methylfuran: 0.03 2-butanone: 0.03 benzene: <0.01 3-buten-2-one: <0.01 2,5-dimethylfuran: 0.07 acetonitrile: 0.04 2,3-butanedione: 0.01 crotonaldehyde: <0.01	n.d.	Gager <i>et al.</i> , 1971b
Sugar, invert	5.42% (w/w)	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of cigarettes (SEB III)	n.d.	n.d.	Concentration/cigarette TPM: 31.6 mg/cig (1.5% ↗) "tar": 27.1 mg/cig (2.0% ↗) water: 2.69 mg/cig (2.5% ↗) nicotine: 1.8 mg/cig (3.6% ↗) acetaldehyde: 1.176 mg/cig (0.6% ↗) acrolein: 108 µg/cig (0.2% ↗) isoprene: 460 µg/cig (9.5% ↗) HCN: 338 µg/cig (8.5% ↗) formaldehyde: 34 µg/cig (22.3% ↗) NO _x : 436 µg/cig (5.8% ↗) CO: 16.1 mL/cig (1.2% ↗) CO ₂ : 32.6 mL/cig (3.3% ↗)	NCI, Report No. 3, 1977

Table 3 (contd.)

Ingredient	Experimental design			Results		Reference(s)	
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products		
Sugar (invert, contd.)					<i>Concentration/g dry condensate</i> indole: 463 µg/g (31.5% ↗) skatole: 315 µg/g (4.7% ↗) B[a]A: 1.41 µg/g (14.6% ↗) B[a]P: 1.02 µg/g (6.4% ↗) o-cresol: 0.70 mg/g (6.9% ↗) m-, p-cresol: 1.93 mg/g (4.5% ↗) tot. w-acids: 2.24 meq/g (0.4% ↗) fatty acids: 21.61 mg/g (8.3% ↗) OLL-acids: 12.92 mg/g (10.1% ↗) palmitic acid: 6.60 mg/g (0.3% ↗) stearic acid: 2.09 mg/g (8.9% ↗) catechol: 5.18 mg/g (5.7% ↗) glycerol: 78.03 mg/g (7.9% ↗) <i>Concentration/cigarette</i> TPM: 28.5 mg/cig (2.2% ↗) "tar": 23.12 mg/cig (1.3% ↗) water: 2.48 mg/cig (9.5% ↗) nicotine: 2.91 mg/cig (18.9% ↗) phenol: 105.95 µg/cig (33.0% ↗) acetaldehyde: 1.05 mg/cig (0.9% ↗) acrolein: 74.88 µg/cig (0.2% ↗) isoprene: 471.87 µg/cig (5.4% ↗) HCN: 326.33 µg/cig (13.0% ↗) formaldehyde: 20.07 µg/cig (10.4% ↗) NO _x : 628.29 µg/cig (11.0% ↗) CO: 11.86 mL/cig (14.8% ↗) CO ₂ : 23.63 mL/cig (16.1% ↗) <i>Concentration/g dry condensate</i> indole: 1427.18 µg/g (18.3% ↗) skatole: 590.3 µg/g (3.1% ↗) B[a]A: 1.22 µg/g (25.6% ↗) B[a]P: 0.82 µg/g (14.6% ↗) o-cresol: 0.51 mg/g (20.3% ↗) m-, p-cresol: 1.98 mg/g (4.2% ↗) colorim. phenols: 5.95 mg/g (0.8% ↗) tot. w-acids: 2.04 meq/g (14.0% ↗) fatty acids: 8.46 mg/g (15.2% ↗) OLL-acids: 4.16 mg/g (15.3% ↗) palmitic acid: 3.09 mg/g (12.5% ↗) stearic acid: 1.21 mg/g (21.9% ↗) neophytadiene: 12.76 mg/g (8.2% ↗) catechol: 3.2 mg/g (1.8% ↗) n.d.		NCI, Report No. 3, 1977
Sugar, invert	5.42% (w/w)	Burley blend	Added during casing ⇒ manufacture of cigarettes (SEB III burley)	n.d.	n.d.		
Sugar, invert	39.1% carbon content	Cigarette	Spraying of cigarettes with labelled ¹⁴ C-invert sugar	n.d.	Carbon ⇒ MSS: gas phase: 13.6% TPM: 9.1%	Jenkins et al., 1980	
Sulfuric acid	40 mg/cig	Tobacco	n.r.	n.r.	smoke-pH: 4.3 (23.2% ↗)	Stedman et al., 1969	

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Thiabendazole	600 ppm	Reconstituted tobacco sheet	n.r.	Estim. value for the thiabendazole transfer into smoke (cigarette weight: 1 g with 20% reconstituted tobacco): 24 µg/cig ⇒ transfer rate: 20%	n.d.	n.d.	Kröller, 1969
Thymol (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Thymol (in γ-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Toluene (in γ-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)
Triacetin	14.9 mg/tip (20 mm)	Cigarette filter	Brush applicator	Delivery of triacetin after 0–8 weeks; the effect of filter ventilation at 25 and 50% dilution is listed as the ratio of vented vs. non-vented delivery	n.d.	n.d.	Mathis, 1983
				Delivery (%) 25% Dilution 50% Dilution 9.1 (0) 0.89 (0) 0.62 (0) 8.5 (1) 0.79 (1) 0.53 (1) 7.7 (2) 0.81 (2) 0.55 (2) 6.8 (4) 0.62 (4) 0.49 (4) 7.0 (6) 0.66 (6) 0.46 (6) 7.6 (8) 0.60 (8) 0.36 (8)			
Triacetin	n.r.	n.r.	n.r.	Sample A: 0.31–0.32 mg/cig Sample B: 0.25–0.33 mg/cig	n.d.	n.d.	Lyerly, 1967
Triethyl orthoformate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 10% ↗ "tar": 13% ↗ nicotine: 43% ↗ phenol: 22% ↗ o-cresol: 5% ↗ m-, p-cresol: 9% ↗ B[a]P: 30% ↗ smoke-pH: 6.8 (21.4% ↗)	Burton and Benner, 1972
Trisodium phosphate	134 mg/cig	Tobacco	n.r.	n.r.	n.r.		Stedman et al., 1969
Trisodium vanadate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	TPM: 22.7% ↗ "tar": 21.2% ↗ nicotine: 46.4% ↗ phenol: 74.6% ↗ o-cresol: 36% ↗ m-, p-cresol: 83.6% ↗ B[a]P: 210.3% ↗	Burton and Benner, 1972
Urea	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.	No evidence of reduction in B[a]P content of smoke	Bentley and Burgan, 1960
Urea	5% (w/w)	Fine-cut tobacco	Spraying of tobacco with a urea containing aqueous solution	n.d.	n.d.	TPM: 5% ↗ B[a]P: 32% ↗ CO: 11% ↗	Pintaske, 1981 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Urea	0.4%	Cigarette blend	n.r.	n.d.	n.d.	NH ₃ : 38 µg/cig (138% ↗) smoke pH: 6.1 (8.9% ↗)	Mariner <i>et al.</i> , 2000 (A)
Vanillin released from: ethyl 3-(4'-butoxy-carbonyloxy-3'-methoxyphenyl)-3-hydroxy-2-phenyl-propanoate	0.01–5% (paper wrapper) 0.0001–5% (filler)	Combustible filler and/or paper wrapper additive	Spraying of an alcoholic solution or injection into the tobacco. Added to tobacco, reconstituted tobacco sheet or cigarette paper	n.r.	vanillin ethyl phenylacetate carbon dioxide isobutene	n.d.	Chan <i>et al.</i> , 1992 (P)
Vanillin released from: 4-t-butoxy-carbonyl-oxy-3-methoxy-benzaldehyde	0.01–5% (paper wrapper) 0.0001–5% (filler)	Combustible filler and/or paper wrapper additive	Spraying of an alcoholic solution or injection into the tobacco. Added to tobacco, reconstituted tobacco sheet or cigarette paper	n.r.	vanillin carbon dioxide isobutene	n.d.	Chan <i>et al.</i> , 1992 (P)
Vanillin	77 µCi/cig (223 µg)	Cigarette	Manual syringe injection of cigarettes with ¹⁴ C-labelled vanillin (53 mCi/mmol)	TPM: 15.9% vapour phase: 0.2%	Extent of decomposition: 0%	n.d.	Green <i>et al.</i> , 1989
Vanillin	1mg	Capillary tube (modelling cigarette combustion)	No application to tobacco	Predicted transfer of vanillin: 100% (200 °C, 2% and 10% O ₂)	No further combustion products	n.d.	Stotesbury <i>et al.</i> , 1999
Vanillin	5000 µg/cig (labelled or unlabelled) or 1 mg (capillary tube)	Cigarette + capillary tube (pyrolysis experiments)	Injection of an ethanolic solution (25 µL) into the cigarette with labelled ¹³ C- and ¹⁸ O-vanillin	Degradation of vanillin at different temperatures 200 °C: 100% (pyrolysis cond.) 200–800 °C: 50.2% (pyrolysis cond.) smoke [¹³ C]: 99.9% Total extent of transfer to the mainstream TPM (intact additive and degradation products): 10.4%	Further combustion products: Smoke [¹³ C] 2-methoxyphenol: 0.1% 200–800 °C phenol: 6.6% 2-methoxyphenol: 6.2% o-cresol: 5.6% 2-hydroxybenzaldehyde: 3% toluene: 2.7%	n.d.	Stotesbury <i>et al.</i> , 2000
Vanillin	1 mg/cig	Cigarette		Transfer rate into MSS: 10% butt: 4%	Increase of o-cresols and phenols by decomposition; phenols ~ 12% of the added vanillin	n.d.	Kato and Shibayama, 1962
Vanillin (in β-cyclodextrine)	n.r.	Tobacco	Spraying	Transfer of aroma to MSS mentioned	n.d.	n.d.	Bavley and Robb, 1969 (P)

Table 3 (contd.)

Ingredient	Experimental design			Results			Reference(s)
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on MSS	
Zeolite Y	4%	Tobacco	Addition of Na-zeolite Y (powder) to cut tobacco (1g) ⇒ manufacture of cigarettes	n.d.	n.d.	<i>Reduction of nitrosamines:</i> NDMA: 5-10% ↗ NNN: 30-36% ↗ NAT: 50-58% ↗ NAB: 45-53% ↗ NNK: 64-72% ↗ <i>Reduction of PAHs:</i> naphthalene: 40-46% ↗ acenaphthalene: 42-50% ↗ anthracene: 52-60% ↗ fluorene: 10-20% ↗ acenaphthene: 10% ↗ <i>No reduction:</i> phenanthrene, B[a]A, chrysene, benzofluoranthene, B[a]P No evidence of reduction in B[a]P content of smoke PAH concentrations in smoke (infra-red arbitrary units): 87 (55.2% ↗)	Meier and Siegmann, 1999
Zinc nitrate	5%	Tobacco	Spraying of an aqueous solution	n.d.	n.d.		Bentley and Burgan, 1960
Zinc oxide	2%	Reconstituted tobacco sheet	Incorporation into a reconstituted tobacco sheet ⇒ manufacture of cigarettes	n.d.	n.d.		Norman <i>et al.</i> , 1973 (P)
Zinc oxide	7.09%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet) SEB III	Added during casing ⇒ manufacture of cigarettes	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 26.34 mg/cig (16.6% ↗) "tar": 22.37 mg/cig (17.5% ↗) water: 2.47 mg/cig (8.2% ↗) nicotine: 1.49 mg/cig (17.2% ↗) phenol: 169.92 µg/cig (3.6% ↗) acetaldehyde: 1.12 mg/cig (4.8% ↗) acrolein: 100.38 µg/cig (7.1% ↗) isoprene: 542.5 µg/cig (17.9% ↗) HCN: 59 µg/cig (82.5% ↗) formaldehyde: 37.6 µg/cig (10.6% ↗) NO_x: 406.41 µg/cig (6.8% ↗) CO_x: 14.89 mL/cig (7.5% ↗) CO₂: 32.86 mL/cig (0.8% ↗) <i>Concentration/g dry condensate</i> indole: 716.3 µg/g (54.7% ↗) skatole: 381.7 µg/g (21.2% ↗) B[a]A: 1.56 µg/g (10.6% ↗) B[a]P: 1.38 µg/g (35.3% ↗) o-cresol: 0.69 mg/g (1.4% ↗) m-, p-cresol: 1.92 mg/g (2.1% ↗) tot. w-acids: 1.92 meq/g (14.3% ↗) fatty acids: 19.28 mg/g (10.8% ↗) OLL-acids: 11.23 mg/g (13.1% ↗) palmitic acid: 5.96 mg/g (9.7% ↗) stearic acid: 2.09 mg/g (0% ↔) catechol: 4.25 mg/g (18.0% ↗) glycerol: 92.0 mg/g (17.9% ↗)	NCI, Report No. 3, 1977

Table 4. Influence of ingredients on the chemical composition of cigarette mainstream smoke (MSS): mixtures

Combination of ingredients	Experimental design			Results			
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	Reference(s)
Sepiolite tobacco waste carboxymethyl-cellulose glycerol phosphoric acid potassium citrate activated carbon (spice, colouring matter) (M 1)	20–40 parts	Reconstituted tobacco sheet	Addition to tobacco sheet (pressing method) ⇒ incorporation into cigarettes	n.d.	n.d.	Reduction of “tar”, B[a]P, CO, and acetone (no data shown)	An <i>et al.</i> , 1996 (P, A)
	30–70 parts						
Water aluminium trihydrate asbestos guar gum glycerol (M 2)	5–8 parts	Reconstituted tobacco sheet	Preparation of a matrix slurry with the ingredients to form a tobacco sheet ⇒ incorporation into cigarettes, containing 23% (w/w) of the sheet	n.d.	n.d.	Sheet, no filter: “tar”: 49% ↗ nicotine: 54% ↗ polonium-210: 41% ↗ Sheet, filter: “tar”: 42% ↗ nicotine: 47% ↗ polonium-210: 35% ↗	Armbrust and Carithers, 1968 (P)
	3–5 parts						
	3–9 parts						
	1–3 parts						
	1–2 parts						
n.r.							
Triacetin glycerol tobacco blend sodium alginate fibre Perlite (M 3)	89 parts	Tobacco blend	Blending with a conventional cut tobacco cigarette filler (3 samples; triacetin and glycerol used in 3 different combinations)	glycerol: 1.11 mg/cig transfer estimated: 1.29% triacetin: 2.03 mg/cig transfer estimated: 2.11%	n.d.	TPM: 7.5; 5.3; 7.6 mg/cig water: 2.7; 0.8; 2.1 mg/cig nicotine: 0.19; 0.1; 0.2 mg/cig NFDPM: 4.59; 4.36; 5.35 mg/cig	Biggs <i>et al.</i> , 1998 (P)
	10 parts						
	1 part						
	0.5 parts						
	0.25 parts						
	0, 9.6, 4% 8.6, 0, 4% 20.3, 20.1, 20%						
	8.1, 8, 8% 1, 1, 1% 62, 61.3, 63%						
Glycerol sorbitol (M 4)	1.7%	Flue-cured blend	Impregnation with an aqueous solution	n.d.	n.d.	flue-cured blend: + 3.4% dry TPM (mg/5 cig): 115 (1.8% ↗)	Bilimoria and Nisbet, 1975
	1.7%						
α-Cellulose calcium carbonate tobacco (cured) potassium citrate sodium citrate disodium hydrogen phosphate sodium bicarbonate inositol glycerol (M 5)	90 g	Reconstituted tobacco sheet (75%) + cured natural tobacco (25%)	Addition of an aqueous solution of ingredients (1.2 mL) to a thermally treated product of α-cellulose and calcium carbonate	n.d.	n.d.	Smoke of cigarettes contains 75% less “tar”, nicotine, PAH's and carbonyl compounds than smoke of cigarettes made of natural tobacco	Briskin, 1979 (P)
	10 g						
	250 mg						
	60 mg						
	12 mg						
	12 mg						
	18 mg						
	30 mg						
	30 mg						

Table 4 (contd.)

Combination of ingredients	Experimental design			Results			Reference
	Amount	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	
Glycerol 1,3-butyleneglycol diethylene glycol propylene glycol triethylene glycol sorbitol (M 6)	1% for each single humectant	Tobacco	Addition of a mixture of the humectants	propylene glycol, 1,3- butylene glycol, diethylene glycol and glycerol were found in MSS	n.r.	n.d.	Carugno <i>et al.</i> , 1971
Magnesium nitrate palladium (M 7)	0.44% 550 ppm	Tobacco	Casing formulation with nitrate and/or palladium	n.d.	n.d.	1.412 mg PAH/g of dry smoke in comparison to the average of 4 controls (37.1% ↗)	Collins <i>et al.</i> , 1981 (P)
Magnesium nitrate palladium (M 8)	0.44% 440 ppm	Tobacco	Casing formulation with nitrate and/or palladium	n.d.	n.d.	1.537 mg PAH/g of dry smoke in comparison to the average of 4 controls (31.5% ↗)	Collins <i>et al.</i> , 1981 (P)
Magnesium nitrate palladium (M 9)	0.46% 550 ppm	Tobacco	Casing formulation with nitrate and/or palladium	n.d.	n.d.	1.272 mg PAH/g of dry smoke in comparison to the average of 4 controls (43.3% ↗)	Collins <i>et al.</i> , 1981 (P)
Methylene chloride cellulose acetate methyl cellulose (highly methylated) tobacco Mica calcium carbonate glycerol propylene glycol 1,3-butyleneglycol methanol (M 10)	360 parts 35 parts 2 parts 38 parts 4.5 parts 4.5 parts 1 part 4 parts 5 parts 40 parts	White envelope for cigarettes	Agitation of the mixture of ingredients to an homogeneous composition ⇒ production of an envelope for heat-sealed cigarettes	n.d.	n.d.	King Size filter cigarette nicotine: 0.74 mg/cig ⇒ 29.5% ↗ "tar": 10.9 mg/cig ⇒ 33.9% ↗ cigarette with cut-off filter nicotine: 0.43 mg/cig ⇒ 4.4% ↗ "tar": 10.65 mg/cig ⇒ 17.6% ↗	Detert and Ruchholz, 1974 (P)
Carboxymethyl-cellulose citric acid titanium dioxide (M 11)	4.3% 1.9% 0.3%	Reconstituted tobacco sheet	Modified Arenco procedure ⇒ manufacture of cigarettes containing 2% diethylene glycol (control) or additives of the tobacco sheet (sheet EA)	n.d.	n.d.	DPM: 32.6 mg/cig (2.1% ↗) nicotine: 1.5 mg/cig (17.1% ↗) phenol: 0.188 mg/cig (2.7% ↗) CO: 22.9 mL/cig (68.4% ↗) NO: ~ 600 ppm (~15.4% ↗) B[a]P: 1.29 ppm (22.9% ↗) acrolein: 58 µg/cig (4.9% ↗) acetaldehyde: 1.83 mg/cig (28.9% ↗) HCN: 0.25 µg/cig (10.7% ↗)	Dontenwill <i>et al.</i> , 1972
Diethylene glycol citric acid glyoxal plasticiser (M 12)	3% 1% 0.4% 2.5%	Reconstituted tobacco sheet	Grinding procedure ⇒ manufacture of cigarettes containing 2% diethylene glycol (control) or additives of the tobacco sheet (sheet EB)	n.d.	n.d.	DPM: 35.2 mg/cig (5.7% ↗) nicotine: 1.57 mg/cig (13.3% ↗) phenol: 0.2 mg/cig (9.3% ↗) CO: 17.5 mL/cig (28.7% ↗) NO: ~ 600 ppm (~15.4% ↗) B[a]P: 1.1 ppm (4.8% ↗) acrolein: 57 µg/ Cig (6.6% ↗) acetaldehyde: 2.01 mg/cig (41.6% ↗) HCN: 0.16 µg/ Cig (42.9% ↗)	Dontenwill <i>et al.</i> , 1972

Table 4 (contd.)

Combination of ingredients	Experimental design			Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	
Methyl cellulose 1,3-butyleneglycol (M 13)	13% 6.7%	Reconstituted tobacco sheet	Mixture of tobacco powder and ingredients ⇒ manufacture of cigarettes containing 2% diethylene glycol (control) or additives of the tobacco sheets (sheet EG ₁)	n.d.	n.d.	DPM: 27.8 mg/cig (16.5% ↗) nicotine: 0.89 mg/cig (50.8% ↗) phenol: 0.034 mg/cig (81.4% ↗) CO: 18.7 mL/cig (37.5% ↗) NO: 580 ppm (11.5% ↗) B[a]P: 0.78 ppm (25.7% ↗) acrolein: 90 µg/cig (47.5% ↗) acetaldehyde: 1.27 mg/cig (10.6% ↗) HCN: 0.19 µg/cig (32.1% ↗)	Dontenwill et al., 1972
Methyl cellulose 1,3-butyleneglycol sodium nitrate (M 14)	12.2% 6.2% 6.6%	Reconstituted tobacco sheet	Mixture of tobacco powder and ingredients ⇒ manufacture of cigarettes containing 2% diethylene glycol (control) or additives of the tobacco sheet (sheet EG ₃)	n.d.	n.d.	DPM: 21.7 mg/cig (34.8% ↗) nicotine: 0.47 mg/cig (74% ↗) phenol: 0.032 mg/cig (82.5% ↗) CO: 13.9 mL/cig (2.2% ↗) NO: 3540 ppm (581% ↗) B[a]P: 0.5 ppm (52.4% ↗) acrolein: 69 µg/cig (13.1% ↗) acetaldehyde: 1.33 mg/cig (6.3% ↗) HCN: 0.22 µg/cig (21.4% ↗)	Dontenwill et al., 1972
Diethylene glycol sorbic acid (M15)	1.5% 0.005%	Reconstituted tobacco sheet	AMF dust impingement procedure ⇒ manufacture of cigarettes containing 2% diethylene glycol (control) or additives of the tobacco sheet (sheet EW)	n.d.	n.d.	DPM: 35.7 mg/cig (7.2% ↗) nicotine: 1.95 mg/cig (7.7% ↗) phenol: 0.2 mg/cig (9.3% ↗) CO: 16.8 mL/cig (23.5% ↗) NO: 650 ppm (25% ↗) B[a]P: 1.05 ppm (↔) acrolein: 29 µg/ cig (52.5% ↗) acetaldehyde: 1.17 mg/cig (17.6% ↗) HCN: 1.5 µg/ cig (436% ↗)	Dontenwill et al., 1972
Diethylene glycol α-cellulose (M 16)	2% 4%	Tobacco and/or tobacco sheet	Production of reconstituted tobacco according to US-Patent 3,298,378 Control cigarette T: 50% Virginia 25% Oriental 25% burley	n.d.	n.d.	Cigarette S (100% sheet): DPM: 22.5 mg/cig (26.7% ↗) nicotine: 1.37 mg/cig (18.9% ↗) phenol: 0.131 mg/cig (26.4% ↗) B[a]P in "tar": 1.3 ppm (6.5% ↗) Cigarette S 50 (50% sheet): DPM: 27.1 mg/cig (11.7% ↗) nicotine: 1.54 mg/cig (8.9% ↗) phenol: 0.161 mg/cig (9.5% ↗) B[a]P in "tar": 1.72 ppm (32.3% ↗) Cigarette SR 20 (20% sheet): DPM: 29 mg/cig (5.5% ↗) nicotine: 1.51 mg/cig (10.6% ↗) phenol: 0.173 mg/cig (2.8% ↗) B[a]P in "tar": 2.14 ppm (54% ↗)	Dontenwill et al., 1976

Table 4 (contd.)

Combination of ingredients	Experimental design			Results		
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components
Diethylene glycol α-cellulose sodium nitrate (M 17)	2%	Tobacco and/or tobacco sheet	Production of reconstituted tobacco according to US-Patent 3,298,378 Control cigarette T: 50% Virginia, 25% Oriental, 25% burley	n.d.	n.d.	Cigarette F (T: 80% + S-sheet: 20% + 1.8% NaNO ₃ + filter): DPM: 13.6 mg/cig (55.7% ↗) nicotine: 0.82 mg/cig (51.5% ↗) phenol: 0.037 mg/cig (80.2% ↗) B[a]P in "tar": 1.43 ppm (2.9% ↗)
Diethylene glycol citric acid glyoxal plasticiser (M 18)	3%	Tobacco	Blend mixture containing: 50% Virginia 25% Oriental 25% burley addition of ingredients: n.r.	n.d.	n.d.	Cigarette B 20 (20% sheet): DPM: 31 mg/cig (1% ↗) nicotine: 1.71 mg/cig (1.2% ↗) phenol: 0.212 mg/cig (19.1% ↗) B[a]P in "tar": 1.5 ppm (7.9% ↗) Cigarette BR 20 (20% sheet of stems): DPM: 30.7 mg/cig (↔) nicotine: 1.7 mg/cig (0.6% ↗) phenol: 0.209 mg/cig (17.4% ↗) B[a]P in "tar": 1.44 ppm (3.6% ↗)
Cellulose sulfate calcium carbonate magnesium iron(III) citrate manganese iron(III) citrate ammonium iron(III) citrate ammonium citrate urea (M 19)	50 g/m ² 50% (w/w)	Tobacco sheet (example A)	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1 ⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	Condensate: 9.4 mg/cig (33.8% ↗) nicotine: 1.35 mg/cig (25% ↗) CO: 12.8 mL/cig (12% ↗)
	100 g/L 30 g/L 30 g/L 60 g/L 50 g/L	Aqueous solution				
Cellulose sulfate calcium carbonate magnesium iron(III) citrate manganese iron(III) citrate ammonium iron(II) citrate ammonium citrate urea (M 20)	50 g/m ² 50% (w/w)	Tobacco sheet (example B)	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1 ⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	Condensate: 8.3 mg/cig (41.5% ↗) nicotine: 1.22 mg/cig (32.2% ↗) CO: 10.9 mL/cig(4% ↗)
	5 g/L 1.5 g/L 1.5 g/L 3 g/L 2.5 g/L	Aqueous solution				
Cellulose sulfate calcium carbonate iron(III) oxide hydrate magnesium iron(III) citrate manganese iron(III) citrate ammonium iron(II) citrate ammonium citrate urea (M 21)	50 g/m ² 50% (w/w) 5% (w/w)	Tobacco sheet (example C)	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1 ⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	Condensate: 8.1 mg/cig (43% ↗) nicotine: 1.19 mg/cig (33.9% ↗) CO: 10.6 mL/cig (6.6% ↗)
	5 g/L 1.5 g/L 1.5 g/L 3 g/L 2.5 g/L	Aqueous solution				

Table 4 (contd.)

Combination of ingredients	Experimental design		Results				
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	Reference
Cellulose sulfate calcium carbonate iron(III) oxide hydrate magnesium iron(III) citrate manganese iron(III) citrate ammonium iron(III) citrate ammonium citrate urea (M 22)	50 g/m ² 50% (w/w) 50 g/L 5 g/L 1.5 g/L 1.5 g/L 3 g/L 2.5 g/L	Tobacco sheet (example 1) Aqueous solution	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	condensate: 7.3 mg/cig (48.6% ↗) nicotine: 1.06 mg/cig (41% ↗) CO: 9.4 mL/cig (17.5% ↗)	Eicher and Müller, 1985 (P)
Cellulose sulfate calcium carbonate iron(III) oxide hydrate iron(III) oxide hydrate magnesium iron(III) citrate manganese iron(III) citrate ammonium iron(III) citrate ammonium citrate urea (M 23)	50 g/m ² 50% (w/w) 5% (w/w) 50 g/L 5 g/L 1.5 g/L 1.5 g/L 3 g/L 2.5 g/L	Tobacco sheet (example 2) Aqueous solution	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	condensate: 7.0 mg/cig (50.7% ↗) nicotine: 1.04 mg/cig (42.4% ↗) CO: 9.7 mL/cig (14.7% ↗)	Eicher and Müller, 1985 (P)
Cellulose sulfate calcium carbonate iron(III) oxide hydrate aluminium oxide hydrate magnesium iron(II) citrate manganese iron(III) citrate 1.0 g/L 2.5 g/L ammonium iron(II) citrate ammonium citrate urea (M 24)	55 g/m ² 43% (w/w) 5% (w/w) 100 g/L 5.5 g/L 1.0 g/L 2.5 g/L 2.0 g/L 2.5 g/L	Tobacco sheet (example 3) Aqueous solution	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	condensate: 7.5 mg/cig (47.2% ↗) nicotine: 1.1 mg/cig (38.8% ↗) CO: 9.4 mL/cig (16.8% ↗)	Eicher and Müller, 1985 (P)
Cellulose sulfate calcium carbonate aluminium oxide hydrate magnesium aluminium citrate (M 25)	50 g/m ² 50% (w/w) 30 g/L 25 g/L	Tobacco sheet (example 4) Aqueous solution	The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	condensate: 7.3 mg/cig (48.6% ↗) nicotine: 1.05 mg/cig (41.7% ↗) CO: 9.8 mL/cig (14% ↗)	Eicher and Müller, 1985 (P)
Cellulose sulfate calcium carbonate titanium dioxide iron(III) chloride sodium phosphate hydrate ammonium iron(III) oxalate (M 26)	50 g/m ² 50% (w/w) 100 g/1.8 L 8.95 g 12.6 g/50 mL 15 g/L	Tobacco sheet (example 5) Aqueous solution	Titanium dioxide + iron(III) chloride ⇒ + sodium phosphate hydrate ⇒ centrifugation ⇒ precipitation ⇒ precipitate + ammonium iron(III) oxalate-solution. The cellulose sulfate sheet was soaked in an aqueous solution containing the substances listed in column 1⇒ production of cigarettes comprising 25 parts sheet and 75 parts tobacco	n.d.	n.d.	condensate: 7.5 mg/cig (47.2% ↗) nicotine: 1.06 mg/cig (41.1% ↗) CO: 9.5 mL/cig (16.7% ↗)	Eicher and Müller, 1985 (P)

Table 4 (contd.)

Combination of ingredients	Experimental design			Results		
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components
Potassium citrate sodium citrate (M 27)	n.r.	Cigarette paper	n.r.	n.d.	n.d.	TPM: 28.1 mg/cig (12.7% ↗) nicotine: 1.51 mg/cig (5.0%)
Momordica grosvenori chlorophyll adipic acid tartaric acid stearic acid gaballon potassium nitrate (M 28)	15–34% 14–30% 10–24% 4–11% 4–15% 3–12% 0.5–4%	Tobacco	n.r.	n.d.	n.d.	Reduction of "tar", nicotine, active oxygen, CO in tobacco smoke (no data)
Lycopodium bisdepuratum (seeds of club moss) potassium nitrate palladium nitrate (M 29)	n.r.	Paper and/ or tobacco	Treatment (e.g. spraying) with 54% aqueous solution of Lycopodium bisdepuratum, 45% KNO ₃ , 1% Pa(NO ₃) ₂	n.d.	n.d.	35% reduction of toxins > 50% reduction of CO is to be expected
Ethyl valerate or menthol zirconium salts or titanium oxide (hydrous) (M 30)	5–80 mg/cig	Filter tip	Insertion between two cellulose acetate filter tips	Release of ethyl valerate or menthol during pyrolysis (no data)	n.d.	"tar": 21 mg (5% ↗) cyanide: 72 µg (11.1% ↗) CO: 11 mg (1.1% ↗) NO _x : 70 µg (14.6% ↗) hydrogen sulfide: 75 µg (21.9% ↗) ammonia: 27 µg (10% ↗) B[a]P: 22 ng (4.8% ↗)
Licorice (spray dried) cocoa sugar glycerol propylene glycol alginate chalk tobacco dust water (M 31)	5 g 5 g 13 g 13 g 10 g 49 g 5 g 270 mL	Tobacco material	Manufacture of a smoke material containing relatively little tobacco material (as dust or extract)	n.d.	n.d.	TPM: 14.8 mg McAdam, 1997 (P)
Licorice (spray dried) cocoa sugar glycerol propylene glycol alginate chalk tobacco extract water (M 32)	5 g 5 g 13 g 13 g 10 g 53g 1 g 245 mL	Tobacco material	Manufacture of a flavour mixture containing relatively little tobacco material	n.d.	n.d.	TPM: 12.9 mg McAdam, 1997 (P)

Jodl, 1969

Komatsu, 1997 (P, A)

Kossack, 1987 (P)

Matsushita and Shinozaki, 1980 (P)

McAdam, 1997 (P)

McAdam, 1997 (P)

Table 4 (contd.)

Combination of ingredients	Experimental design			Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	
Licorice (spray dried) cocoa sugar glycerol propylene glycol alginate chalk tobacco extract (synth. analogue) water (M 33)	5 g 5 g 13 g 13 g 10 g 53.5 g 0.5 g 250 mL	Tobacco material	Manufacture of a flavour mixture containing relatively little tobacco material	n.d.	n.d.	TPM: 10.4 mg	McAdam, 1997 (P)
Licorice (spray dried) cocoa sugar glycerol propylene glycol alginate chalk tobacco dust water (M 34)	5 g 5 g 13 g 13 g 10 g 49 g 5 g 340 mL	Tobacco material	Manufacture of a flavour mixture containing relatively little tobacco material	n.d.	n.d.	TPM: 11.4 mg	McAdam, 1997 (P)
Carboxymethylcellulose dolomitic limestone (M 35)	25% 25%	Tobacco	Manufacture of a smoking composition containing 50% tobacco, 25% carboxymethyl-cellulose (CMC) and 25% dolomitic limestone (dry mixture)	n.d.	n.d.	dry "tar": 13.7 mg/cig (44.8% ↗) acetaldehyde: 27.2 µg/puff (43.1% ↗) acetonitrile: 5.0 µg/puff (69.9% ↗) acrolein: 2.5 µg/puff (56.9% ↗) furan: 1.1 µg/puff (64.5% ↗) propionaldehyde: 1.8 µg/puff (57.1% ↗) acetone: 15.6 µg/puff (44.7% ↗) propionitrile: 0.9 µg/puff (66.7% ↗) isobutyraldehyde: 0.8 µg/puff (63.6% ↗) benzene: 3.4 µg/puff (52.1% ↗)	Miano and Keith, 1976 (P)
Carboxymethylcellulose dolomitic limestone carbon wetting agent plasticiser colorant (M 36)	37% 37% 10% 16% n.r. n.r.	Tobacco	Manufacture of a 50:50 blend of tobacco and the film or a 50:50 blend of tobacco and the synthetic material	n.d.	n.d.	<i>Film (50:50)</i> methanol: 5.7 µg/puff (55.5% ↗) acetaldehyde: 46.7 µg/puff (2.3% ↗) acetonitrile: 8.6 µg/puff (48.2% ↗) acrolein: 4.3 µg/puff (25.9% ↗) furan: 1.9 µg/puff (38.7% ↗) propionaldehyde: 5.6 µg/puff (36.6% ↗) acetone: 22.4 µg/puff (20.6% ↗) propionitrile: 1.1 µg/puff (59.3% ↗) isobutyraldehyde: 1.3 µg/puff (40.9% ↗) benzene: 4.8 µg/puff (32.4% ↗) <i>Dry mixed (50:50)</i> methanol: 5.9 µg/puff (53.9% ↗) acetaldehyde: 34.9 µg/puff (27% ↗) acetonitrile: 6.1 µg/puff (63.3% ↗) acrolein: 3.8 µg/puff (34.5% ↗) furan: 1.45 µg/puff (53.2% ↗) propionaldehyde: 2.0 µg/puff (51.2% ↗) acetone: 15.8 µg/puff (44% ↗) propionitrile: 0.8 µg/puff (70.4% ↗) isobutyraldehyde: 1.0 µg/puff (54.5% ↗) benzene: 2.7 µg/puff (62% ↗)	Miano and Keith, 1976 (P)

Table 4 (contd.)

Combination of ingredients	Experimental design			Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	
Carboxymethylcellulose dolomitic limestone carbon wetting agent plasticiser colorant (M 37)	37% 37% 10% 16% n.r. n.r.	Tobacco	Manufacture of a 50:50 blend of tobacco and the film	n.d.	n.d.	cyanide: 83 µg/cig (63.1% ↗) phenol: 39 µg/cig (38.1% ↗) CO: 3.1 vol.% (8.4% ↗) B[a]P: 2.4 µg/100 cig (↔)	Miano and Keith, 1976 (P)
Anisole benzaldehyde menthol estragole β-damascenone ambroxide γ-undecalactone vanillin (M 38)	n.r.	Cigarette		Determination of the flavour percentage transferred to the vapour and particulate phase of MSS	n.d.		Miranda et al., 1999 (A)
Sodium hydroxide titanyl chloride wood pulp (M 39)	7% 7.5%	Reconstituted tobacco sheet of whole SEB-1 (experimental cigarette)	"Schweitzer process" for tobacco sheet production. Addition of titanil chloride to the fibrous part and wood pulp to the fiber slurry	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 15.95 mg/cig (13.3% ↗) water: 1.89 mg/cig (4.1% ↗) nicotine: 0.78 mg/cig (12.4% ↗) "tar": 13.28 mg/cig (14.5% ↗) acetaldehyde: 885 µg/cig (7.8% ↗) acrolein: 104.9 µg/cig (0.9% ↗) formaldehyde: 32.1 µg/cig (31.7% ↗) HCN: 143.1 µg (42.1% ↗) NO _x : 403.7 µg/cig (0.6% ↗) CO: 14.43 mL/cig (2.6% ↗) CO ₂ : 21.39 mL/cig (15.6% ↗) <i>Concentration/g dry condensate</i> phenol: 6 mg/g (85.2% ↗) o-cresol: 1.06 mg/g (58.2% ↗) <i>m</i> -, <i>p</i> -cresol: 2.49 mg/g (71.7% ↗) colorim. phenols: 7.99 mg/g (46.9% ↗) tot. w-acids: 2.67 meq/g (1.8% ↗) phenanthrene: 27.3 µg/g (46.0% ↗) B[a]A: 1.44 µg/g (41.2% ↗) B[a]P: 0.98 µg/g (88.5% ↗) <i>Concentration in % (w/w) TPM</i> palmitic acids: 0.25% (3.8% ↗) OLL-acids: 0.39% (11.4% ↗) stearic acids: 0.13% (7.1% ↗) fatty acids: 0.77% (8.3% ↗)	NCI, Report No.1., 1976

Table 4 (contd.)

Combination of ingredients	Experimental design			Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	
Ethylhydroxyethyl cellulose methocel sulfite pulp (M 40)	1.84% 7.35% 4.59%	Reconstituted tobacco sheet	Production of reconstituted tobacco sheet (slurry process, medium density) with and without additives	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 31.35 mg/cig (11.4% ↗) water: 3.52 mg/cig (6.1% ↗) nicotine: 1.42 mg/cig (28.3% ↗) "tar": 26.58 mg/cig (11.5% ↗) acetaldehyde: 1298 µg/cig (11.88% ↗) acrolein: 132.1 µg/cig (53.4% ↗) formaldehyde: 31.1 µg/cig (22.5% ↗) HCN: 119.9 µg/cig (37.1% ↗) NO _x : 421.3 µg/cig (28.0% ↗) CO: 23.31 mL/cig (5.3% ↗) CO ₂ : 29.49 mL/cig (21.4% ↗) <i>Concentration/g dry condensate</i> phenol: 2.67 mg/g (37.0% ↗) o-cresol: 0.44 mg/g (29.0% ↗) m-, p-cresol: 1.04 mg/g (45.5% ↗) colorim. phenols: 4.10 mg/g (37.9% ↗) tot. w-acids: 2.07 meq/g (3.7% ↗) phenanthrene: 14.1 µg/g (31.9% ↗) B[a]A: 0.91 µg/g (13.3% ↗) B[a]P: 0.64 µg/g (24.7% ↗) <i>Concentration in % (w/w) TPM</i> palmitic acids: 0.29% (17.1% ↗) OLL-acids: 0.51% (15.0% ↗) stearic acids: 0.15% (0% ↗) fatty acids: 0.95% (13.6% ↗)	NCI, Report No. 1, 1976
Glycerol sugar, invert (M 41)	2.8% 5.3%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇔ manufacture of experimental cigarettes (SEB III)	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 31.6 mg/cig (13.7% ↗) "tar": 27.1 mg/cig (12.5% ↗) water: 2.69 mg/cig (28.7% ↗) nicotine: 1.8 mg/cig (10.4% ↗) phenol: 164 µg/cig (3.8% ↗) acetaldehyde: 1.176 mg/cig (5.7% ↗) acrolein: 108 µg/cig (7.7% ↗) isoprene: 460 µg/cig (13.6% ↗) HCN: 338 µg/cig (13.3% ↗) formaldehyde: 34 µg/cig (0.8% ↗) NO _x : 436 µg/cig (1.0% ↗) CO: 16.1 mL/cig (0.5% ↗) CO ₂ : 32.6 mL/cig (4.9% ↗)	NCI, Report No. 3, 1977

Table 4 (contd.)

Combination of ingredients	Experimental design		Results		Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Glycerol sugar, invert (M 41) (contd.)					<i>Concentration/g dry condensate</i> indole: 463 µg/g (36.4% ↗) skatole: 315 µg/g (8.3% ↗) BlajA: 1.41 µg/g (16.5% ↗) BlajP: 1.02 µg/g (2.0% ↗) o-cresol: 0.70 mg/g (2.9% ↗) m-, p-cresol: 1.93 mg/g (2.5% ↗) tot. w-acids: 2.24 mg/g (6.7% ↗) fatty acids: 21.61 mg/g (7.1% ↗) OLL-acids: 12.92 mg/g (6.5% ↗) palmitic acid: 6.60 mg/g (5.2% ↗) stearic acid: 2.09 mg/g (15.4% ↗) catechol: 5.18 mg/g (12.8% ↗) glycerol: 78.03 mg/g (control: 0 mg)
Glycerol sugar, invert magnesium nitrate (M 42)	2.6% 5.0% 5.7%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of experimental cigarettes (SEB III)	n.d.	n.d. <i>Concentration/cigarette</i> TPM: 33.39 mg/cig (20.1% ↗) "tar": 27.99 mg/cig (16.2% ↗) water: 3.77 mg/cig (80.4% ↗) nicotine: 1.63 mg/cig (0% ↗) phenol: 199.92 µg/cig (26.6% ↗) acetaldehyde: 1.32 mg/cig (18.7% ↗) acrolein: 133.38 µg/cig (33.0% ↗) isoprene: 546.25 µg/cig (2.6% ↗) HCN: 510.5 µg/cig (71.2% ↗) formaldehyde: 34.5 µg/cig (2.3% ↗) NO_x: 1379 µg/cig (213.1% ↗) CO: 17.65 mL/cig (916% ↗) CO₂: 38.25 mL/cig (23.1% ↗) <i>Concentration/g dry condensate</i> indole: 439.8 µg/g (39.6% ↗) skatole: 303.2 µg/g (11.7% ↗) BlajA: 1.43 µg/g (18.2% ↗) BlajP: 1.21 µg/g (21.0% ↗) o-cresol: 0.52 mg/g (23.5% ↗) m-, p-cresol: 1.61 mg/g (18.7% ↗) colorim. phenols: 5.36 mg/g (24.7% ↗) tot. w-acids: 2.12 mg/g (11.7% ↗) fatty acids: 21.25 mg/g (8.6% ↗) OLL-acids: 12.83 mg/g (7.2% ↗) palmitic acid: 6.23 mg/g (10.5% ↗) stearic acid: 2.10 mg/g (15.0% ↗) neophytadiene: 9.64 mg/g (3.5% ↗) catechol: 4.74 mg/g (20.2% ↗) glycerol: 72.2 mg/g (control: 0 mg)

NCI, Report No.
3, 1977

Table 4 (contd.)

Combination of ingredients	Experimental design		Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components
Glycerol sugar, invert zinc oxide (M 43)	2.6% 4.9% 7.09%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇌ manufacture of experimental cigarettes (SEB III)	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 26.34 mg/cig (5.3% ↗) "tar": 22.37 mg/cig (7.1% ↗) water: 2.47 mg/cig (18.2% ↗) nicotine: 1.49 mg/cig (8.6% ↗) phenol: 169.92 µg/cig (7.6% ↗) acetaldehyde: 1.12 mg/cig (0.7% ↗) acrolein: 100.38 µg/cig (0.1% ↗) isoprene: 542.5 µg/cig (1.9% ↗) HCN: 59 µg/cig (80.2% ↗) formaldehyde: 37.6 µg/cig (11.5% ↗) NO_x: 406.41 µg/cig (7.7% ↗) CO: 14.89 mL/cig (8.0% ↗) CO₂: 32.86 mL/cig (5.8% ↗) <i>Concentration/g dry condensate</i> indole: 716.3 µg/g (1.6% ↗) skatole: 381.7 µg/g (11.2% ↗) B[a]A: 1.56 µg/g (28.9% ↗) B[a]P: 1.38 µg/g (38.0% ↗) o-cresol: 0.69 mg/g (1.5% ↗) m-, p-cresol: 1.92 mg/g (3.0% ↗) colorim. phenols: 6.71 mg/g (5.8% ↗) tot. w-acids: 1.92 mg/g (20.0% ↗) fatty acids: 19.28 mg/g (17.1% ↗) OLL-acids: 11.23 mg/g (18.7% ↗) palmitic acid: 5.96 mg/g (14.4% ↗) stearic acid: 2.09 mg/g (15.4% ↗) neophytadiene: 9.98 mg/g (0.1% ↗) catechol: 4.25 mg/g (18.5% ↗) glycerol: 92.0 mg/g (control: 0 mg)
Glycerol sugar, invert magnesium nitrate zinc oxide (M 44)	2.45% 4.61% 5.61% 6.96%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇌ manufacture of experimental cigarettes (SEB III)	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 25.57 mg/cig (8.0% ↗) "tar": 22.34 mg/cig (7.3% ↗) water: 2.08 mg/cig (0.5% ↗) nicotine: 1.14 mg/cig (30.1% ↗) phenol: 102.0 µg/cig (35.4% ↗) acetaldehyde: 1.238 mg/cig (11.3% ↗) acrolein: 131.38 µg/cig (31.1% ↗) isoprene: 457.5 µg/cig (14.1% ↗) HCN: 93.38 µg/cig (68.7% ↗) formaldehyde: 39.47 µg/cig (17.1% ↗) NO_x: 1407 µg/cig (219.6% ↗) CO: 14.27 mL/cig (11.8% ↗) CO₂: 32.5 mL/cig (4.6% ↗)

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Table 4 (contd.)

Combination of ingredients	Experimental design		Results		
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Glycerol sugar, invert magnesium nitrate zinc oxide (M 44) (contd.)					<i>Concentration/g dry condensate</i> indole: 545.1 µg/g (25.2% ↗) skatole: 360.4 µg/g (5.0% ↗) B[a]A: 1.44 µg/g (19.0% ↗) B[a]P: 1.17 µg/g (17.0% ↗) o-cresol: 0.53 mg/g (22.1% ↗) m-, p-cresol: 1.58 mg/g (20.2% ↗) colorim. phenols: 6.04 mg/g (15.2% ↗) tot. w-acids: 1.72 meq/g (28.3% ↗) fatty acids: 19.34 mg/g (16.8% ↗) OLL-acids: 10.94 mg/g (20.8% ↗) palmitic acid: 5.86 mg/g (15.8% ↗) stearic acid: 2.03 mg (17.8% ↗) neophytadiene: 10.52 mg/g (5.3% ↗) catechol: 3.6 mg/g (39.4% ↗) glycerol: 70.9 mg/g (control: 0 mg) <i>Concentration/cigarette</i> TPM: 25.57 mg/cig (19.1% ↗) "tar": 22.34 mg/cig (17.6% ↗) water: 2.08 mg/cig (22.7% ↗) nicotine: 1.14 mg/cig (36.7% ↗) phenol: 102.0 µg/cig (37.8% ↗) acetaldehyde: 1.238 mg/cig (5.3% ↗) acrolein: 131.38 µg/cig (21.6% ↗) isoprene: 457.5 µg/cig (0.5% ↗) HCN: 93.38 µg/cig (35.4% ↗) formaldehyde: 39.47 µg/cig (16.1% ↗) NO_x: 1407 µg/cig (222.7% ↗) CO: 14.27 mL/cig (11.4% ↗) CO₂: 32.5 mL/cig (0.3% ↗) <i>Concentration/g dry condensate</i> indole: 545.1 µg/g (17.7% ↗) skatole: 360.4 µg/g (14.4% ↗) B[a]A: 1.44 µg/g (2.1% ↗) B[a]P: 1.17 µg/g (14.7% ↗) o-cresol: 0.53 mg/g (24.3% ↗) m-, p-cresol: 1.58 mg/g (18.1% ↗) tot. w-acids: 1.72 meq/g (23.2% ↗) fatty acids: 19.34 mg/g (10.5% ↗) OLL-acids: 10.94mg/g (15.3% ↗) palmitic acid: 5.86 mg/g (11.2% ↗) stearic acid: 2.03 mg/g (2.9% ↗) catechol: 3.6 mg/g (30.5% ↗) glycerol: 70.9 mg/g (9.1% ↗)
Magnesium nitrate zinc oxide (M 45)	5.61% 6.96%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of experimental cigarettes (SEB III)	n.d.	n.d.

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Table 4 (contd.)

Combination of ingredients	Experimental design		Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components
Cellulose ether gums dialdehyde crosslinker galacto-mannan gums sulfite pulp (M 46)	{0.52% 0.58% 5.85% 6.05%} ⇒ 13%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of experimental cigarettes (SEB IV) made from reconstituted tobacco sheet: "AMF"- slurry process + galacto-mannan gums + cellulose ether gums + sulfite pulp (unbleached) + dialdehyde crosslinker	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 25.57 mg/cig (19.1% ↗) "tar": 22.34 mg/cig (17.6% ↗) water: 2.08 mg/cig (22.7% ↗) nicotine: 1.14 mg/cig (36.7% ↗) phenol: 102.0 µg/cig (37.8% ↗) acetaldehyde: 1.238 mg/cig (5.3% ↗) acrolein: 131.38 µg/cig (21.6% ↗) isoprene: 457.5 µg/cig (0.5% ↗) HCN: 93.38 µg/cig (35.4% ↗) formaldehyde: 39.47 µg/cig (16.1% ↗) NO _x : 1407 µg/cig (222.7% ↗) CO: 14.27 mL/cig (11.4% ↗) CO ₂ : 32.5 mL/cig (0.3% ↗) <i>Concentration/g dry condensate</i> indole: 545.1 µg/g (17.7% ↗) skatole: 360.4 µg/g (14.4% ↗) B[a]A: 1.44 µg/g (2.1% ↗) B[a]P: 1.17 µg/g (14.7% ↗) o-cresol: 0.53 mg/g (24.3% ↗) m-, p-cresol: 1.58 mg/g (18.1% ↗) tot. w-acids: 1.72 meq/g (23.2% ↗) fatty acids: 19.34 mg/g (10.5% ↗) OLL-acids: 10.94 mg/g (15.3% ↗) palmitic acid: 5.86 mg/g (11.2% ↗) stearic acid: 2.03 mg/g (2.9% ↗) catechol: 3.6 mg/g (30.5% ↗) glycerol: 70.9 mg/g (9.1% ↗)
Cellulose ether gums citric acid dialdehyde crosslinker galacto-mannan gums sodium hydroxide sulfite pulp (M 47)	{0.52% 2.8% 0.58% 5.85% 3.2% 6.05%} ⇒ 19%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of experimental cigarettes (SEB IV) made from reconstituted tobacco sheet: "AMF"- slurry process + galacto-mannan gums + cellulose ether gums + sulfite pulp (unbleached) + dialdehyde crosslinker + citric acid + sodium hydroxide	n.d.	n.d.	<i>Concentration/cigarette</i> TPM: 26.7 mg/cig (21.5% ↗) "tar": 23.1 mg/cig (19.8% ↗) water: 3.21 mg/cig (5.9% ↗) nicotine: 0.36 mg/cig (79.2% ↗) phenol: 109 µg/cig (9.1% ↗) acetaldehyde: 803 µg/cig (19.5% ↗) acrolein: 93 µg/cig (14.7% ↗) isoprene: 321 µg/cig (18.1% ↗) HCN: 248 µg/cig (33.7% ↗) formaldehyde: 58 µg/cig (45.0% ↗) NO _x : 349 µg/cig (39.7% ↗) CO: 22.0 mL/cig (15.1% ↗) CO ₂ : 31.3 mL/cig (23.1% ↗)

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Table 4 (contd.)

Combination of ingredients	Experimental design		Results		Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products
Cellulose ether gums citric acid di-aldehyde crosslinker galacto-mannan gums sodium hydroxide sulfite pulp (M 47) (contd)					<i>Concentration/g dry condensate</i> indole: 260 mg/g (39.0% ↗) skatole: 438 mg/g (26.6% ↗) B[a]A: 0.83 µg/g (22.4% ↗) B[a]P: 0.69 µg/g (13.7% ↗) o-cresol: 0.58 mg/g (41.5% ↗) <i>m</i>-, <i>p</i>-cresol: 1.52 mg/g (6.2% ↗) colorim. phenols: 6.5 mg/g (23.3% ↗) tot. w-acids: 2.38 mg/g (2.5% ↗) fatty acids: 15.91 mg/g (16.2% ↗) OLL-acids: 7.75 mg/g (20.8% ↗) palmitic acid: 5.21 mg/g (15.4% ↗) stearic acid: 2.95 mg/g (3.6% ↗) neophytadiene: 5.27 mg/g (37.6% ↗) glycerol: 77.6 mg/g (23.9% ↗) catechol: 5.42 mg/g (5.2% ↗)
Cellulose calcium carbonate clay (M 48)	10% 18% 7%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of experimental cigarettes (SEB IV made from reconstituted tobacco sheet: "Schweitzer" paper process) + additives	n.d.	<i>Concentration/cigarette</i> TPM: 17.9 mg/cig (28.7% ↗) "tar": 13.3 mg/cig (32.8% ↗) water: 3.53 mg/cig (16.0% ↗) nicotine: 1.06 mg/cig (10.2% ↗) phenol: 52 µg/cig (21.2% ↗) acetaldehyde: 480 µg/cig (43.4% ↗) acrolein: 65 µg/cig (46.3% ↗) isoprene: 82 µg/cig (69.5% ↗) HCN: 2158 µg/cig (13.7% ↗) formaldehyde: 17 µg/cig (46.9% ↗) NO_x: 314 µg/cig (44.7% ↗) CO: 12.2 mL/cig (29.5% ↗) CO₂: 26.6 mL/cig (1.5% ↗) <i>Concentration/g dry condensate</i> indole: 170 mg/g (20.6% ↗) skatole: 208 mg/g (24.1% ↗) B[a]A: 1.60 µg/g (122.2% ↗) B[a]P: 1.11 µg/g (91.4% ↗) o-cresol: 0.67 mg/g (24.1% ↗) <i>m</i>-, <i>p</i>-cresol: 1.33 mg/g (8.9% ↗) colorim. phenols: 4.8 mg/g (19.1% ↗) tot. w-acids: 2.00 mg/g (34.4% ↗) fatty acids: 12.33 mg/g (14.5% ↗) OLL-acids: 5.32 mg/g (8.1% ↗) palmitic acid: 4.23 mg/g (32.2% ↗) stearic acid: 2.79 mg/g (57.6% ↗) neophytadiene: 2.25 mg/g (51.9% ↗) glycerol: 151 mg/g (31.3% ↗) catechol: 5.41 mg/g (1.3% ↗)

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n.d.

Table 4 (contd.)

Combination of ingredients	Experimental design		Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components
Cellulose ether gums diethylene crosslinker galacto-mannan gums sulfite pulp	{0.52% 0.58% 5.85% 6.05%} ⇒ 13%	Tobacco blend (flue-cured, burley, Maryland, Turkish, reconstituted sheet)	Added during casing ⇒ manufacture of experimental cigarettes (SEB IV) made from reconstituted tobacco sheet: "AMF"- slurry process + galacto-mannan gums + cellulose ether gums + sulfite pulp (unbleached) + diethylene crosslinker	n.d.	n.d.	Concentration/cigarette TPM: 2.5 mg/cig (92.6% ↗) "tar": 1.9 mg/cig (93.4% ↗) water: 0.51 mg/cig (85.0% ↗) nicotine: 0.09 mg/cig (94.8% ↗) phenol: 34 µg/cig (71.9% ↗) acetaldehyde: 304 µg/cig (69.5% ↗) acrolein: 71 µg/cig (34.9% ↗) isoprene: 76 µg/cig (80.6% ↗) HCN: 0 µg/cig (100.0% ↗) formaldehyde: 10 µg/cig (75.0% ↗) NO _x : 174 µg/cig (69.9% ↗) CO: 4.4 mL/cig (83.0% ↗) CO ₂ : 19.9 mL/cig (51.1% ↗) Concentration/g dry condensate indole: 8.2 mg/g (98.1% ↗) skatole: 56 mg/g (83.8% ↗) B[a]A: 3.34 µg/g (212.1% ↗) B[a]P: 1.78 µg/g (122.5% ↗) o-cresol: 0.17 mg/g (58.5% ↗) m-, p-cresol: 0.43 mg/g (73.5% ↗) colorim phenols: 1.45 mg/g (72.5% ↗) tot. w-acids: 2.20 meq/g (9.8% ↗) fatty acids: 17.19 mg/g (9.5% ↗) OLL-acids: 7.65 mg/g (21.8% ↗) palmitic acid: 5.67 mg/g (8.0% ↗) stearic acid: 3.87 mg/g (26.5% ↗) neophytadiene: 3.17 mg/g (62.5% ↗) glycerol: 170 mg/g (66.7% ↗) catechol: 3.15 mg/g (38.8% ↗)
calcium carbonate (CaCO ₃) (M 49)	60%					NCI, Report No. 4, 1980)
Palladium salts magnesium nitrate (M 50)	0.06% (NH ₄) ₂ PdCl ₆ or (NH ₄) ₂ PdCl ₄ + 0.55% Mg(NO ₃) ₂	Reconstituted tobacco sheet	Palladium salt and magnesium nitrate incorporation into a reconstituted tobacco sheet	n.d.	n.d.	Norman and Bryant, 1975 (P)
Ascorbic acid stearic acid citric acid maltose comfrey powder potassium nitrate powder of rhizome glycyrrhizae radix perfume humectant (M 51)	n.r.	Cigarette blend	n.r.	n.r.	n.r.	Ogawa, 1998 (P)

Table 4 (contd.)

Combination of ingredients	Experimental design			Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components	
Ascorbic acid chlorophyll citrus fruit or herb (M 52)	n.r.	Attached to the tip of tobacco or mixed in shredded leaves	n.r.	n.r.	n.r.	Reduction of "tar" and nicotine	Ohshiro, 1999 (P)
Calcium alginate cellulose potassium nitrate Flavor C 146 FD and C 1956 Brown (M 53)	80% 10% 5% 1% 2.5%	Reconstituted tobacco sheet	Addition of tobacco (55% or less) to the sheet material	n.r.	n.r.	Cigarettes sheet (50% substitute + 50% tobacco): dry-TPM 15.3 mg/cig (48.8% ↘) Cigarettes sheet + filter (50% substitute + 50% tobacco): dry-TPM 12.7 mg/cig (39.5% ↘)	Prouse <i>et al.</i> , 1977 (P)
Diammonium phosphate sucrose (M 54)	n.r.	Cigarette blend		n.r.	n.d.	Determination of ammonia, carbonyl compounds, pyrazines, nicotine in smoke and smoke "pH"	Saint-Jalm <i>et al.</i> , 2000 (A)
Menthol propylene glycol glycerol (M 55)	n.r.	Tobacco	n.r.	n.r.	n.d.	n.d.	Settle <i>et al.</i> , 1999 (A)
Glucose fructose (M 56)	17.8%	Burley tobacco	Spraying with aqueous sugar solutions	n.d.	n.d.	TPM: 35 mg/cig (2.9% ↗) alkaloids: 1.98 mg/cig (40.4% ↗) carbonyls: 4.5 mg/cig (12.5% ↗) volatile carbonyls: 2.2 mg/cig (15.8% ↗) volatile aldehydes: 0.54 mg/cig (10% ↗) 2-furfural: 90 µg/cig (69.8% ↗) total acids: 2.52 mg/cig (7.2% ↗) volatile acids: 1.16 mg/cig (10.5% ↗)	Thornton and Massey, 1975
Sucrose menthol (M 57)	3 and 5% sucrose 6 and 5% menthol	Filter (activated carbon)	Carbon was impregnated by immersion in sucrose solution. Menthol added by equilibration in a desiccator	menthol (8 puffs of 35 mL): n.d. sucrose (5%): no filter: 0.39 mg/cig filter: 0.46 mg/cig sucrose (3%): no filter: 0.42 mg/cig filter: 0.55 mg/cig	n.d.	n.d.	Tiggelbeck and Manes, 1976 (P)
1-Octanol 1-decanol (M 58)	480 ppm	Tobacco	Spraying (1:1 mixture)	n.d.	n.d.	wet TPM: 40.1 mg/cig (9.1% ↗) dry TPM: 36 mg/cig (10.2% ↗) nicotine: 3.32 mg/cig (12.6% ↗) volatile phenols: 195 µg/cig (21.3% ↗) B[a]P: 4.71 µg/100 g tobacco (12.1% ↗) B[a]A: 6.97 µg/100 g tobacco (9.6% ↗)	Tso, 1975 (P)

Table 4 (contd.)

Combination of ingredients	Experimental design		Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	
Ingredient group 1 (casing materials, volatile top flavourings and ingredients incorporated in reconstituted tobacco sheet) (M 62)	High level concentrations	Test cigarettes (designed to match an industry standard and to be representative of a type of cigarette sold around the world)	Construction of cigarettes with conventional commercial equipment (in a manner similar to 1R4F)	n.d.	n.d.	Carmines, 2002 ^b
Influence on other MSS components						
TPM: 9.74 mg/cig (13.1% ↗)						
nicotine: 0.76 mg/cig (2.7% ↗)						
water: 0.63 mg/cig (26% ↗)						
CO: 11.4 mg/cig (14% ↗)						
NO _x : 0.268 mg/cig (1.9% ↗)						
HCN: 145.5 mg/cig (80.1% ↗)						
formaldehyde: 19.1 mg/cig (15.8% ↗)						
acetaldehyde: 551 mg/cig (6.4% ↗)						
acrolein: 54.5 mg/cig (17.7% ↗)						
phenol: 11.79 mg/cig (↔)						
o-cresol: 3.29 mg/cig (0.6% ↘)						
m-cresol: 2.7 mg/cig (5.9% ↗)						
p-cresol: 6.32 mg/cig (0.6 ↘)						
catechol: 54.3 mg/cig (0.9% ↗)						
resorcinol: 1.13 mg/cig (36.1% ↗)						
hydroquinone: 48.4 mg/cig (11.8% ↗)						
vinyl chloride: 0.032 mg/cig (6.7% ↗)						
1,3-butadiene: 44.3 mg/cig (3.7% ↗)						
isoprene: 346 mg/cig (8.5% ↗)						
acrylonitrile: 10.4 mg/cig (14.9% ↗)						
benzene: 46.2 mg/cig (16.1% ↗)						
toluene: 86.4 mg/cig (28.6% ↗)						
naphthalene: 319 ng/cig (15.6% ↗)						
B[a]P: 5.73 ng/cig (12.4% ↗)						
NPYR: 10 ng/cig (20% ↗)						
NNN: 115 ng/cig (7.3% ↗)						
NAT: 91.6 ng/cig (12.7% ↗)						
NAB: 14.3 ng/cig (23.1% ↗)						
NNK: 130 ng/cig (5.8% ↗)						
cadmium: 34.7 ng/cig (40.5% ↗)						
lead: 12.9 ng/cig (27.7% ↗)						
arsenic: 3.0 ng/cig (9.9% ↗)						

Table 4 (contd.)

Combination of ingredients	Experimental design		Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	Influence on other MSS components
Ingredient Group 2 (casing materials and volatile top flavourings) (M 63)	High level concentrations	Test cigarettes (designed to match an industry standard and to be representative of a type of cigarette sold around the world)	Construction of cigarettes with conventional commercial equipment (in a manner similar to 1R4F)	n.d.	n.d.	TPM: 11.01 mg/cig (27.9% ↗) nicotine: 0.67 mg/cig (9.5% ↗) water: 1.24 mg/cig (148% ↗) CO: 12.3 mg/cig (14% ↗) NO _x : 0.265 mg/cig (23% ↗) HCN: 104 µg/cig (28.7% ↗) formaldehyde: 15.1 µg/cig (8.5% ↗) acetaldehyde: 557 µg/cig (7.5% ↗) acrolein: 52.5 µg/cig (13.4% ↗) phenol: 4.61 µg/cig (60.9% ↗) o-cresol: 1.49 µg/cig (55% ↗) <i>m</i> -cresol: 1.26 µg/cig (50.6% ↗) <i>p</i> -cresol: 3.07 µg/cig (51.7% ↗) catechol: 40.3 µg/cig (25.1% ↗) resorcinol: 0.74 µg/cig (10.8% ↗) hydroquinone: 35 µg/cig (19.2% ↗) vinyl chloride: 0.032 µg/cig (6.7% ↗) 1,3-butadiene: 47.5 µg/cig (11.2% ↗) isoprene: 373 µg/cig (16.9% ↗) acrylonitrile: 8.93 µg/cig (1.9% ↗) benzene: 46.3 µg/cig (16.3% ↗) toluene: 83.3 µg/cig (24.7% ↗) naphthalene: 165 ng/cig (40.2% ↗) B[a]P: 5.31 ng/cig (4.1% ↗) NPYR: 10.5 ng/cig (16% ↗) NNN: 115 ng/cig (7.3% ↗) NAT: 91.4 ng/cig (12.9% ↗) NAB: 13.2 ng/cig (29% ↗) NNK: 117 ng/cig (15.2% ↗) cadmium: 34.0 ng/cig (37.7% ↗) lead: 14.5 ng/cig (43.6% ↗) arsenic: 2.8 ng/cig (15.9% ↗)

Carmines, 2002^b

Table 4 (contd.)

Combination of ingredients	Experimental design		Results			Reference
	Amount ^a	Application to	Method of application	Transfer to MSS (unchanged)	Pyrolysis products	
Ingredient Group 3 (casing materials and menthol) (M 64)	High level concentrations	Test cigarettes (designed to match an industry standard and to be representative of a type of cigarette sold around the world)	Construction of cigarettes with conventional commercial equipment (in a manner similar to 1R4F)	n.d.	n.d.	Carmines, 2002 ^b
Influence on other MSS components						
TPM: 10.03 mg/cig (16.5% ↗)						
nicotine: 0.69 mg/cig (6.8% ↗)						
water: 0.5 mg/cig (↔)						
CO: 10.8 mg/cig (8% ↗)						
NO _x : 0.255 mg/cig (3% ↗)						
HCN: 97.7 µg/cig (20.9% ↗)						
formaldehyde: 27.2 µg/cig (64.8% ↗)						
acetaldehyde: 525 µg/cig (1.4% ↗)						
acrolein: 47 µg/cig (1.5% ↗)						
phenol: 10.6 µg/cig (10.1% ↗)						
o-cresol: 2.95 µg/cig (10.9% ↗)						
m-cresol: 2.42 µg/cig (5.1% ↗)						
p-cresol: 6.1 µg/cig (4.1% ↗)						
catechol: 53 µg/cig (5.1% ↗)						
resorcinol: 1.4 µg/cig (68.7% ↗)						
hydroquinone: 41.2 µg/cig (4.8% ↗)						
vinyl chloride: 0.028 µg/cig (6.7% ↗)						
1,3-butadiene: 38.7 µg/cig (9.4% ↗)						
isoprene: 295 µg/cig (7.5% ↗)						
acrylonitrile: 8.1 µg/cig (10.5% ↗)						
benzene: 39.8 µg/cig (↔)						
toluene: 71.7 µg/cig (6.7% ↗)						
naphthalene: 205 ng/cig (25.7% ↗)						
B[a]P: 5.56 ng/cig (9% ↗)						
NPYR: 9.9 ng/cig (20.8% ↗)						
NNN: 103 ng/cig (16.9% ↗)						
NAT: 83.3 ng/cig (20.6% ↗)						
NAB: 13.7 ng/cig (26.4% ↗)						
NNK: 116 ng/cig (15.9% ↗)						
cadmium: 34.7 ng/cig (40.5% ↗)						
lead: 13 ng/cig (28.7% ↗)						
arsenic: 3.53 ng/cig (6% ↗)						

^aData refer to the amount of single ingredients within the mixture or within the relevant end product, respectively.^bCarmines, 2002: stands on behalf of the following series of publications: Carmines, 2002; Römer *et al.*, 2002; Rustemeier *et al.*, 2002 and Vanscheeuwijck *et al.*, 2002.

Table 5: Pyrolysis experiments with tobacco ingredients

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Acetic acid (sodium salt)	50 g (in 0.5 g portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	Acetic acid (present)	<i>PAH</i> : none <i>Quinones</i> : none <i>Phenols</i> : none <i>Others</i> : acetic acid anhydride	Kröller, 1966b
Agar-agar	30 g (in 0.5–1.0 g portions) of the additive were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable (because a complex mixture or a polymerized product was investigated)	<i>PAH</i> : pentacene, coronene, B[a]P 47 µg/100 g, fluoranthene, anthracene, tetrabenzonaphthalene, fluorene, acenaphthene <i>Quinones</i> : toluolquinone, anthraquinone <i>Phenols</i> : <i>o</i> -cresol, pyrogallol <i>Others</i> : aliphatic hydrocarbons, water, CO ₂ , (formic acid, acetic acid)	Kröller, 1965b
Agar-agar	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products</i> : acetoin, methyl formate, 3-methylfuran, 2-methyl-2-cyclopentene-1-one, furfural, acetylacetone, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, isomaltol, 2-furanmethanol, cyclooctane, 3-methyl-2-hydroxycyclopentenone, hydroxyfuranone isomer, methyl-3-furanecarboxylate, phenol, 4-oxopentanoic acid, 4-methyl-4-hepten-3-one, acetic acid, propionic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985
Alginate acid	30 g (in 0.5–1.0 g portions) of the additive were heated at 700 °C for about 10 min (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : B[a]P 3 µg/100 g, anthracene, chrysene, 4,5-methylenepheneanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : 3,5-ethylenedimethylphenol, ethylphenol, carvacrol, 2,4,6-trimethylphenol, <i>p</i> -cresol, β-naphthol, pyrogallol <i>Others</i> : aliphatic and olefinic hydrocarbons, water, CO ₂ , formaldehyde, acetic acid	Kröller, 1965b
Alginate acid	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products</i> : methyl formate, 3-methylfuran, 2-methyl-2-cyclopenten-1-one, furfural, acetylacetone, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, isomaltol, 2-furanmethanol, cyclooctane, 3-methyl-2-hydroxycyclopentenone, hydroxyfuranone isomer, methyl-3-furanecarboxylate, phenol, benzyl alcohol derivative, 4-oxopentanoic acid, furanecarboxylic acid derivative, 4-methyl-4-hepten-3-one, acetic acid, propionic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985
Anethole (as Diels-Alder adduct with maleic anhydride)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	anethole 14%	n.d.	Robb <i>et al.</i> , 1964
Benzoic acid (sodium salt)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	benzoic acid (present)	<i>PAH</i> : B[a]P, B[a]P 20 µg/100 g, fluoranthene, 2,3-benzofluorene, acenaphthylene, 5,12-dihydrotetracene, dimethylbenzanthracene, terphenyl, 2-methylphenanthrene <i>Quinones</i> : anthraquinone, acenaphthenequinone <i>Phenols</i> : <i>p</i> -benzylphenol, <i>p</i> -cresol, <i>o</i> -ethylphenol <i>Others</i> : aliphatic hydrocarbons, monocarboxylic acids	Kröller, 1970

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Buckthorne berry extract (from <i>Rhamnus cartharticus</i>) major components: rhamnetin rhamnecicin	3 g of extract were heated at 700 °C for 1 h in an air flow of 1.5 L/min	not applicable	water, acetic acid, catechol, guajacol, <i>m</i> -cresol, α -naphthol, β -naphthol, pyrogallol, pyrene, fluoranthene, B[a]P 2 µg/100 g extract. B[a]P content insignificant compared to that in tobacco smoke	Kröller, 1963a
1,3-Butylene glycol	2 mL of the glycol on silica were heated at 700 °C for about 10 min (until the glycol has disappeared) in an air flow of 1.5 L/min	36%	<i>PAH</i> : B[a]P about 13 µg/100 g, fluoranthene, 2-methylphenanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>o</i> - and <i>p</i> -cresol <i>Others</i> : hydrocarbons, CO ₂ , water, aldehydes	Kröller, 1964b
1,3-Butylene glycol	Pyrolysis of 100 g of polyalcohol was investigated at various temperatures	not applicable	<i>Principal compounds at 600 °C</i> : formaldehyde, acetaldehyde 10–15 g/100 g	Doihara <i>et al.</i> , 1964
Campeachy wood extract (from <i>Haematoxylon campe-chianum</i>), major components: Haematein	3 g of extract were heated at 700 °C for 40 min in an air flow of 1.5 L/min	not applicable	CO, CO ₂ , water, formaldehyde, acetic acid, phenol, <i>m</i> -cresol, catechol, anthraquinone, fluoranthene, phenanthrene, B[a]P < 1 µg/100 g extract, traces of: 4,5-methylenephenanthrene, pyrene, naphthacene, pyrenequinone amounts of carcinogens insignificant compared to those in tobacco smoke	Kröller, 1963b
Carboxymethyl-cellulose sodium salt	30 g (in 0.5 g portions) of the cellulose derivate were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : perylene, phenanthrene, 1,2-fluoranthene, B[a]P 12 µg/100 g, benzanthracene 2 µg/100 g, anthracene, 20-methylcholanthrene 1 µg/100 g <i>Quinones</i> : phenanthrenequinone, anthraquinone <i>Phenols</i> : phenol, <i>o</i> -cresol, carvacrol, pyrogallol, gallic acid, catechol <i>Others</i> : aliphatic hydrocarbons, aldehydes, carboxylic acids, water	Kröller, 1964a
Carboxymethyl-cellulose	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products</i> : acetoin, methyl formate, 3-methylfuran, 2-methyl-2-cyclopenten-1-one, furfural, acetylacetone, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, isomaltol, 2-furanmethanol, decanoic acid, cyclooctane, 3-methyl-2-hydroxycyclopentenone, hydroxyfuranone isomer, methyl-3-furanecarboxylate, phenol, benzyl alcohol derivative, 4-oxopentanoic acid, furanecarboxylic acid derivative, 4-methyl-4-hepten-3-one, acetic acid, propionic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid	Sjöberg and Pyysalo, 1985
Carboxymethyl starch	30 g (in 0.5 g portions) of the additive were heated at 700 °C for up to 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : 1,2-benzanthracene, B[a]P 30 µg/100 g, fluoranthene, phenanthrene, anthracene, 2-methylphenanthrene <i>Quinones</i> : phenanthrenequinone, anthraquinone <i>Phenols</i> : phenol, <i>o</i> -cresol, guajacol, <i>o</i> -ethylphenol, pyrogallol, gallic acid, catechol <i>Others</i> : aliphatic hydrocarbons, aldehydes, carboxylic acids, water	Kröller, 1966a
5-Carboxyvanillin	Compound pyrolysed in helium at 300 °C	vanillin 92.0%	CO ₂ : 4.5% 5-carboxy-3,4-dimethoxybenzaldehyde: 3.5%	Southwick, 1992 (P)

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Carob (locust bean gum)	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products:</i> acetoin, methyl formate, furfural, 3-methylfuran, 2-furanmethanol, acetylacetone, cyclooctane, 2-methyl-2-cyclopenten-1-one, isomaltol, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, phenol, 3-methyl-2-hydroxycyclopentenone, methyl-3-furanecarboxylate, hydroxyfuranone isomer, benzyl alcohol derivative, 4-oxopentanoic acid, furanecarboxylic acid derivative, 4-methyl-4-hepten-3-one, acetic acid, propionic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985
Carob seed powder (from <i>Ceratonia siliqua</i> L.)	30 g (in 0.5–1.0 g portions) of the additive were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH:</i> pentacene, coronene, B[a]P 6 µg/100 g, fluoranthene, 2,3-benzofluorene, anthracene <i>Quinones:</i> anthraquinone, benzoquinone <i>Phenols:</i> phenol, <i>o</i> -cresol, pyrogallol <i>Others:</i> aliphatic hydrocarbons, water, formaldehyde, formic acid	Kröller, 1965b
Casein	Pyrolysis of 0.5–2.0 g at 800–860 °C in an N ₂ -flow	not applicable	<i>Principle products:</i> pyridine, quinoline, pyrrole, toluene, phenol, <i>m</i> -, <i>p</i> -cresol <i>Other products:</i> 2-methylpyridine, 3-/4-methylpyridine, 3-vinylpyridine, aniline, isoquinoline, benzene, styrene, xylene, benzonitrile, indene, <i>o</i> -tolunitrile, <i>m</i> -tolunitrile, naphthalene, indole, fluorene, <i>o</i> -cresol, ethylphenol, xylene	Schmeltz <i>et al.</i> , 1972
Casein	About 1 g of material was heated to 840 ± 10 °C in a stream of nitrogen (60 mL/min)	n.d.	<i>Selected pyrolysis products:</i> benzene 9.0%, indole 6.8%, pyridine 23.0%, quinone 13.4%, phenol 35.3%	Higman, E.B. <i>et al.</i> , 1970
Cellobiose	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g): phenol 31, <i>o</i> -cresol 9, <i>m</i> -, <i>p</i> -cresol 11	Schlotzhauer <i>et al.</i> , 1967
Cellubiose	15–30 mg of material was heated to 250, 350, 500 °C for 5, 1 and 1 min, respectively in a stream of helium (60 mL/min)	n.d.	<i>Relative amounts (cm peak height for 10 mg) of selected pyrolysis products at 500 °C:</i> acetaldehyde 10.0, propionaldehyde 1.3, acrolein 2.6, furfural 4.8	Kato, 1967
Cellulose	<i>Condition 1: air, 100 mL/min</i> 314 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 3: air, 100 mL/min</i> 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 4: N₂, 100 mL/min</i> 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	n.d.	<i>Condition 1:</i> 0.024% phenol <i>Condition 3:</i> 0.008% phenol <i>Condition 4:</i> 0.04% phenol	Bell <i>et al.</i> , 1966
Cellulose (from cotton)	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g): phenol 6, <i>o</i> -cresol 2, <i>m</i> -, <i>p</i> -cresol 2	Schlotzhauer <i>et al.</i> , 1967
Cellulose	0.2–0.5 mg cellulose (filter paper untreated and nitrate-treated) were pyrolysed for 30 s at 400–800 °C (50 °C intervals) in nitrogen and air	not applicable	<i>Major pyrolysis products at 500 °C (mg/g cellulose):</i> <i>In N₂ (neat) – N₂ + KNO₃ – air</i> acetaldehyde: 4.7 – 3.0 – 15.7 acrolein: 8.1 – 3.9 – 20.8 3-buten-2-one: 4.0 – 1.5 – 3.7 glucopyranose: 5.3 – 3.0 – 7.7 5-hydroxymethyl-2-furaldehyde: 10.0 – 2.0 – 7.8	Sakuma <i>et al.</i> , 1981
Cellulose	0.5 g of cellulose were heated at 700 °C for 5–6 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH:</i> picene, B[a]P ~8 µg/100 g, fluoranthene, anthracene, 4,5-methylenephenanthrene <i>Quinones:</i> phenanthrenequinone, anthraquinone, pyrenequinone <i>Phenols:</i> pyrogallol, <i>m</i> -cresol <i>Others:</i> hydrocarbons, water, CO ₂ , formaldehyde, acetic acid	Kröller, 1964a

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Cellulose	5–10 mg cellulose were heated for 10 s at 700 °C under an N ₂ -flow (15 mL/min)	n.d.	2-furaldehyde 20.7%, 3-hydroxy-2-methylpyran-4-one 10.0%, 5-methyl-2-furaldehyde 2.1%, 3-methylfuran 6.1%, furancarboxylic acid methyl ester 6.9%, 3-methyl-2,4(3 <i>H</i> ,5 <i>H</i>)-furanone 5.1%, 2-furanmethanol 2.0%, 1,3-cyclopentanone 3.6%, propionic acid methyl ester 1.1%	Schlottzauer <i>et al.</i> , 1985
Cellulose	Cellulose was rapidly heated (within 2 min) to 300–550 °C in a stream of helium at flow rates of 100, 200 and 300 cm ³ /min	n.d.	Condition with maximum yields (450 °C and 100 cm ³ /min): hydrogen 46.0 µmol/L, methane 42.6 µmol/L, carbon monoxide 660.0 µmol/L, ethene 15.4 µmol/L, ethane 2.36 µmol/L, propene 4.36 µmol/L, carbon dioxide 168.0 µmol/L, propene 0.2 µmol/L, but-1-ene 0.0 µmol/L, butane 0.24 µmol/L	Cullis <i>et al.</i> , 1983b
Cellulose	Cellulose was rapidly heated (within 2 min) to 300–550 °C in a stream of nitrogen with increasing amounts of oxygen (5–21 vol.%) at a flow rate of 100 cm ³ /min	n.d.	Condition with almost maximum yields (450 °C and 100 cm ³ /min nitrogen with 21% oxygen): hydrogen 838 µmol/L, methane 1315 µmol/L, carbon monoxide 9483 µmol/L, ethene 648 µmol/L, propene 141 µmol/L, carbon dioxide 4547 µmol/L, oxygen 676 µmol/L, nitrogen 27397 µmol/L	Cullis <i>et al.</i> , 1983a
Cellulose	5 g of material was rapidly heated to 650 °C in a stream of nitrogen for 1 h	n.d.	PAHs (out of 11 investigated)(µg/100 g): pyrene 219, B[a]P 78	Gilbert and Lindsey, 1957
Cellulose	About 1 g of material was heated to 840 ± 10 °C in a stream of nitrogen (60 mL/min)	n.d.	<i>Selected pyrolysis products:</i> benzene 25.7%, furfural —, pyrene 2.1%, phenol 67.5%, B[a]P 288.8 µg/g	Higman, E.B. <i>et al.</i> , 1970
Cellulose	15–30 mg of material was heated to 250, 350, 500 °C for 5, 1 and 1 min, respectively in a stream of helium (60 mL/min)	n.d.	<i>Relative amounts (cm peak height for 10 mg) of selected pyrolysis products at 500 °C:</i> acetaldehyde 11.4, propionaldehyde 2.6, acrolein 1.9, furfural 3.3	Kato, 1967
Cellulose	5 g/30 min cellulose were pyrolysed at various temperatures (350–880 °C) in a stream of nitrogen (85–1050 mL/min)	n.d.	<i>Influence on pyrolytic B[a]P formation:</i> Temperature: increase with temp., sharp increase at 650 °C <i>Oxygen:</i> higher yield in the presence of O ₂ <i>Metals, salts:</i> strong effect (decrease) of iron, nickel, cobalt, ferric oxide, ferrocene moderate effect of nitrate <i>Flow rate of carrier gas:</i> increase with flow <i>Atmosphere:</i> nitric oxide inhibits, propene increases B[a]P yield	Robb <i>et al.</i> , 1966
Cellulose	25 g material were pyrolysed at 800 °C in the following way: 12 cycles consisting of an "operative time" (20 s in a gas flow of nitrogen and air [1 L/min for each gas], simulating a puff) followed by an "inoperative time" (40 s in a flow of nitrogen, simulating the puff interval)	n.d.	<i>Major pyrolysis products (catechols):</i> furfural 5.4 mg/g, levoglucosan 2.9 mg/g	Schlottzauer <i>et al.</i> , 1982
Cellulose monoacetate	30 g (in portions) of the cellulose derivate were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH:</i> naphthacene, B[a]P 28.5 µg/100 g, fluoranthene, anthracene, 20-methylcholanthrene <i>Quinones:</i> toluolquinone, naphthoquinone, anthraquinone <i>Phenols:</i> pyrogallol, o-cresol, 3,5-ethyl-methyl-phenol <i>Others:</i> acetic acid, aliphatic hydrocarbons, water, aldehyde(s)	Kröller, 1964a

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Chlorogenic acid	25 g material were pyrolysed at 800 °C in the following way: 12 cycles consisting of an "operative time" (20 s in a gas flow of nitrogen and air [1 L/min for each gas], simulating a puff) followed by an "inoperative time" (40 s in a flow of nitrogen, simulating the puff interval)	n.d.	<i>Major pyrolysis products (catechols):</i> catechol: 43.3 mg/g, 4-ethylcatechol 40.2 mg/g, phenol 13.9 mg/g, 5-(hydroxymethyl)furfural 13.2 mg/g	Schlotzhauer <i>et al.</i> , 1982
Citric acid	5 g of material was rapidly heated to 650 °C in a stream of nitrogen for 1 h	n.d.	PAHs (out of 11 investigated): pyrene 24 µg/100 g, B[a]P 17 µg/100 g	Gilbert and Lindsey, 1957
Citric acid (sodium salt)	50 g (in 0.5 g portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH:</i> 1,2,5,6-dibenzanthracene, coronene, B[a]P 5 µg/100 g, fluoranthene, 20-methylcholanthrene <i>Quinones:</i> anthraquinone <i>Phenols:</i> phenol, pyrogallol <i>Others:</i> aliphatic hydrocarbons, carboxylic acids, CO, CO ₂ , water	Kröller, 1966b
Cocoa	20 g were pyrolysed at 350, 450, 550, 650 and 750 °C	not applicable	<i>Formation of phenol, o-cresol, m-, p-cresol, xlenols, catechol (between 0.001 and 0.085% at all temperatures tested)</i> <i>Palmitic acid:</i> 0.334% (350 °C), 0.355% (450 °C), 0.184% (550 °C), 0.052% (650 °C) <i>Stearic acid:</i> 0.538% (350 °C), 0.593% (450 °C), 0.309% (550 °C), 0.086% (650 °C)	Schlotzhauer, 1978
Collagen	Pyrolysis of 0.5–2.0 g at 800–860 °C in an N ₂ -flow	not applicable	<i>Principle products:</i> pyridine, 2-methylpyridine, 3-/4-methylpyridine, pyrrole, phenol <i>Other products:</i> 3-vinylpyridine, aniline, quinoline, isoquinoline, benzene, toluene, styrene, xylene, benzonitrile, indene, o-tolunitrile, m-tolunitrile, naphthalene, indole, m-, p-cresol, ethylphenol, xlenol	Schmeltz <i>et al.</i> , 1972
Collagen	About 1 g of material was heated to 840 ± 10 °C in a stream of nitrogen (60 mL/min)	n.d.	Selected pyrolysis products: benzene 0.6%, indole 7.2%, pyridine 26.5%, quinone 7.6%, phenol 19.6%	Higman <i>et al.</i> , 1970
Cyclodextrins	Cyclodextrins mixed with 3 times its weight of Celite and pyrolysed at 750 °C, for 1 min in a stream of nitrogen (15–25 mL/min)	n.d.	<i>Identified:</i> methanol, ethylene, acetaldehyde, acetone, acrolein, 3-methyl-1-butene, furan, 2-methylfuran <i>Provisionally identified:</i> methane, ethane, propane, propene, propionaldehyde, 1-butene, 2-methylbutene-1, n-butane, butadiene, 2,3-butanedione, 2-butanone, pentane, 1-hexane	Robb <i>et al.</i> , 1964
Cyclopentadiene (as Diels-Alder adduct with acetylene-dicarboxylic acid)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	cyclopentadiene 26%	n.d.	Robb <i>et al.</i> , 1964
Deertongue leaf powder	5.2 g (in 1 g portions) were pyrolysed at 840 ± 10 °C under nitrogen	not applicable	<i>Neutrals (0.22 g):</i> benzene 7.0%, toluene 15.4%, styrene 1.0%, benzofuran 8.7%, indene 6.1%, naphthalene 4.4%, methyl-naphthalene 13.5%, coumarin/acenaphthene 8.0%, phenanthrene/anthracene 2.4%, methylphenanthrene/anthracene 5.6% <i>Nitrogen bases (0.02 g):</i> pyridine 3.4%, picoline 6.3%, dimethylpyridine 4.9%, vinylpyridine 5.1%, indole 1.3%, quinoline 8.1%, isoquinoline 3.5%, methylquinoline 6.9%, carbazole 1.0%, benzoquinoline 1.1%, methylbenzoquinoline 2.1% <i>Phenols (0.005 g):</i> phenol 15.5%, cresol 20.2%, xlenol 3.6%, coumarin 1.3%, naphthol 2.8%	Higman <i>et al.</i> , 1974

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
<i>endo</i> -Dehydronorborneol	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	cyclopentadiene 17%	acetaldehyde 12%, benzene 1%	Robb <i>et al.</i> , 1964
Dextrin	5–10 mg dextrin were heated for 10 s at 700 °C under an N ₂ -flow (15 mL/min)	n.d.	3-methylfuran 19.9%, 2-furaldehyde 16.7%, 1,3 cyclopentanedione 6.2%, 2-furanmethanol 3.8%, cyclopentanone 2.8%, propionic acid methyl ester 2.5%, 2-hydroxy-3-methyl-2-cyclopenten-1-one 2.1%, 2-methyl-2-cyclopenten-1-one 2.0%, 2,4-pentanedione 1.8%, 5-methyl-2-furaldehyde 1.7%	Schlotzhauer <i>et al.</i> , 1985
Dialdehyde starch (Oxystarch)	30 g (in 0.5 g portions) of the additive were heated at 700 °C for up to 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : pentacene, B[a]P 23.5 µg/100 g, fluoranthene, phenanthrene, terphenyl <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>m</i> -cresol <i>Others</i> : aliphatic hydrocarbons, formaldehyde, acetic acid, water	Kröller, 1966a
Dibutyl phthalate	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : 1,2,5,6-dibenzanthracene, naphthacene, pyrene, anthracene, B[a]P 12 µg/100 g <i>Quinones</i> : anthraquinone <i>Phenols</i> : phenol, <i>m</i> -xyleneol <i>Others</i> : phthalic acid anhydride, <i>n</i> -butanol, aliphatic hydrocarbons, CO ₂	Kröller, 1968
Diethylene glycol	2 mL of the glycol on silica were heated at 700 °C for about 10 min (until the glycol has disappeared) in an air flow of 1.5 L/min	77%	<i>PAH</i> : fluoranthene, naphthacene, B[a]P ~1.5 µg/100 g <i>Quinones</i> : anthraquinone <i>Phenols</i> : none <i>Others</i> : aldehydes	Kröller, 1964b
Docosane	<i>Condition 3: air, 100 mL/min</i> 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 4: N₂, 100 mL/min</i> 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	n.d.	Condition 3: 0.022% phenol Condition 4: 0% phenol	Bell <i>et al.</i> , 1966
Ethyl 2-(2-butyl)-3-hydroxy-3-methyl-3-phenylpropionate	10 mg of the ester were pyrolysed in an open tube at 250 °C for 5 min	n.d.	>90% decomposition to a 1:1 mixture of acetophenone + ethyl valerate	Grubbs and Houminer, 1982 (P)
Ethyl vanillyl-D-glucoside	Pyrolysis in a thermal analyzer in the thermogravimetric mode (50–900 °C)	mass loss of 66.5% at 226 °C is consistent with levoglucosan formation and ethyl vanillin release	n.d.	Herron, 1988 (P)
Flavour mixture (brown, aromatic taste)	50 g (in portions) of the flavour material on silica were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : B[a]P 1 µg/100 g, fluoranthene, phenanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>o</i> -cresol, pyrogallol <i>Others</i> : aliphatic hydrocarbons, formaldehyde, vanillin, essential oils	Kröller, 1967
Fructose	5 g of material was rapidly heated to 650 °C in a stream of nitrogen for 1 h	n.d.	<i>PAHs</i> (out of 11 investigated): pyrene 35 µg/100 g, B[a]P 33 µg/100 g	Gilbert and Lindsey, 1957
Fructose	About 1 g of material was heated to 840 ± 10 °C in a stream of nitrogen (60 mL/min)	n.d.	<i>Selected pyrolysis products</i> : benzene 27.4%, furfural 12.5%, pyrene 0.13%, phenol 77.9%, B[a]P 98.4 µg/g	Higman <i>et al.</i> , 1970
Fructose	25 g material were pyrolysed at 800 °C in the following way: 12 cycles consisting of an "operative time" (20 s in a gas flow of nitrogen and air [1 L/min for each gas], simulating a puff) followed by an "inoperative time" (40 s in a flow of nitrogen, simulating the puff interval)	n.d.	<i>Major pyrolysis products (catechols)</i> : furfural 38.6 mg/g, 5-hydroxymethylfurfural 19.5 mg/g	Schlotzhauer <i>et al.</i> , 1982
Furan (as Diels-Alder adduct with acetylene-dicarboxylic acid)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	furan 33%	n.d.	Robb <i>et al.</i> , 1964

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Glucose	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	n.d.	Formation of phenols (mg/100 g): phenol 27, <i>o</i> -cresol 7, <i>m</i> -, <i>p</i> -cresol 5	Schlottzhauer <i>et al.</i> , 1967
Glucose	Condition 1: air, 100 mL/min 314 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace) Condition 2: air, 100 mL/min 520 °C (furnace 1) 530 °C (furnace 2) 685 °C (mobile furnace) Condition 3: air, 100 mL/min 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) Condition 4: N ₂ , 100 mL/min 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	n.d.	Condition 1: 0.050% phenol Condition 2: 0.061% phenol Condition 3: 0.077% phenol Condition 4: 0.090% phenol	Bell <i>et al.</i> , 1966
Glucose	Pyrolysis of glucose at 200–500 °C (reported here are only results obtained at 450–500 °C)	n.d.	Composition of gases: CO ₂ : 9.27%, CO: 35.22%, C _n H _{2n} : 0.73%, CH ₄ : 43.55%, H ₂ : 11.91%	Tomasik, 1989
Glucose	5 g of material was rapidly heated to 650 °C in a stream of nitrogen for 1 h	n.d.	PAHs (out of 11 investigated): pyrene: 66 µg/100 g, B[a]P: 29 µg/100 g	Gilbert and Lindsey, 1957
Glucose	About 1 g of material was heated to 840 ± 10 °C in a stream of nitrogen (60 mL/min)	n.d.	Selected pyrolysis products: benzene 17.6%, pyrene —, furfural 7.4%, phenol 59.6%, B[a]P 47.5 µg/g	Higman <i>et al.</i> , 1970
Glucose	15–30 mg of material was heated to 250, 350, 500 °C for 5, 1 and 1 min, respectively in a stream of helium (60 mL/min)	n.d.	Relative amounts (cm peak height for 10 mg) of selected pyrolysis products at 500 °C: acetaldehyde 5.6, propionaldehyde 1.5, acrolein 4.3, furfural 3.3	Kato, 1967
Glucuronic acid	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g) phenol 18, <i>o</i> -cresol 4, <i>m</i> -, <i>p</i> -cresol 5	Schlottzhauer <i>et al.</i> , 1967
Glycerol	Pyrolysis of glycerol in a steam with argon as purge gas at 650–700 °C	650 °C: 82.4% 675 °C: 66% 700 °C: 75%	Mol-% of converted glycerol at 650/675/700 °C acrolein: 52/39/34 acetaldehyde: 48/38/42 CO: —/35/58 hydrogen: —/29/44 ethylene: —/10/17 methane: —/ 5/11 ethane: —/1/2 CO ₂ : —/0.3/1	Stein and Antal, 1983
Glycerol	Pyrolysis of 100 g of the polyalcohol was investigated at various temperatures	not applicable	Principal compounds at 600 °C acetaldehyde 10–15 g/100 g, acrolein < 0.5 g/100 g	Doihara <i>et al.</i> , 1964
Glycerol	30 g (in portions) of the humectant on silica were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	60%	PAH: tribenzopyrene, pentacene, coronene, B[a]P 6 µg/100 g, fluoranthene, anthracene Quinones: anthraquinone Phenols: phenol Others: aldehyde(s), carboxylic acids, aliphatic hydrocarbons, water, CO ₂	Kröller, 1965a
Glycine	Pyrolysis of 0.5–2.0 g at 800–860 °C in an N ₂ -flow	not applicable	Pyridine, 2-methylpyridine, pyrrole, toluene, indene	Schmeltz <i>et al.</i> , 1972
Glycyrrhizic acid	2 mg pyrolysed in a Curie-point pyrolyser 770 °C for 12.5 s under nitrogen (40 mL/min)	n.d.	18 Compounds identified, major components: 2,5-dimethylfuran, 2(3H)-furanone, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-ol, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-one, pentamethyloctahydro-naphthalene	Yongkuan and Wangyun, 1995

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Glycyrrhizic acid disodium salt	2 mg pyrolysed in a Curie-point pyrolyser 770 °C for 12.5 s under nitrogen (40 mL/min)	n.d.	38 Compounds identified, major components: 2,5-dimethylfuran, 2(3 <i>H</i>)-furanone, pentamethyloctahydronaphthalene, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-one, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-ol disodium glycyrrhetate is optimum Asweetener@	Yongkuan and Wangyun, 1995
Glycyrrhizic acid monosodium salt	2 mg pyrolysed in a Curie-point pyrolyser 770 °C for 12.5 s under nitrogen (40 mL/min)	n.d.	18 Compounds identified, major components: pentamethyldecahydronaphthalene, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-one, 2,5-cyclohexadien-1-one, 2(3 <i>H</i>)-furanone, 2,5-dimethylfuran, tetramethylhexahydronaphthalene	Yongkuan and Wangyun, 1995
Glycyrrhizic acid trisodium salt	2 mg pyrolysed in a Curie-point pyrolyser 770 °C for 12.5 s under nitrogen (40 mL/min)	n.d.	36 Compounds identified, major components: pentamethyloctahydronaphthalene, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-one, 3,4-dimethyl-4-ethyl-2,5-cyclohexadien-1-ol, 1,4,6-trimethyldihydronaphthalene, trimethyltetrahydronaphthalene	Yongkuan and Wangyun, 1995
Glyoxal	30 g (in portions) of the additive on silica were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : B[a]P 3.4 µg/100 g, fluoranthene, 2,3-benzofluorene <i>Quinones</i> : none <i>Phenols</i> : <i>o</i> -cresol <i>Others</i> : aliphatic hydrocarbons, carboxylic acids	Kröller, 1970
Guar gum	30 g (in 0.5–1.0 g portions) of the additive were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : pentacene, phenanthrene, fluoranthene, coronene, 1,2,5,6-dibenzanthracene, B[a]P 30 µg/100 g, terphenyl <i>Quinones</i> : acenaphthenequinone, phenanthrenequinone, anthraquinone <i>Phenols</i> : phenol, <i>m</i> -cresol, gallic acid, catechol <i>Others</i> : aliphatic hydrocarbons, water, CO ₂ , formic acid, acetic acid	Kröller, 1965b
Guar gum	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products</i> : acetoin, methyl formate, 2-methyl-2-cyclopenten-1-one, 3-methylfuran, furfural, acetylacetone, isomaltol, 2,4-hexadienal, 5-methyl-2-furfural, 2-furylmethylketone, 2-furanmethanol, cyclooctane, furanecarboxylic acid derivative, hydroxyfuranone isomer, methyl-3-furanecarboxylate, 3-methyl-2-hydroxycyclopentenone, phenol, benzyl alcohol derivative, 4-methyl-4-hepten-3-one, acetic acid, propionic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985
Guar, oxygenated	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : B[a]P 15 µg/100 g, hexahydropyrene, fluoranthene <i>Quinones</i> : none <i>Phenols</i> : <i>m</i> -cresol, catechol, pyrogallol <i>Others</i> : aldehydes, acetic acid, aliphatic hydrocarbons, water	Kröller, 1968
Gummi arabicum	30 g (in 0.5–1.0 g portions) of the additive were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : pentacene, 1,2,5,6-dibenzanthracene, coronene, B[a]P 32 µg/100 g, fluoranthene, terphenyl, phenanthrene, dihydropyrene <i>Quinones</i> : phenanthrenequinone, anthraquinone <i>Phenols</i> : phenol, <i>m</i> -cresol, gallic acid <i>Others</i> : aliphatic hydrocarbons, water, acetic acid	Kröller, 1965b

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Gummi arabicum	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products:</i> acetoin, methyl formate, furfural, 3-methylfuran, isomaltol, 2-methyl-2-cyclopenten-1-one, acetylacetone, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, 2-furanmethanol, cyclooctane, furanecarboxylic acid derivative, 2-methylpropionic acid, 3-methyl-2-hydroxycyclopentenone, hydroxyfuranone isomer, phenol, benzyl alcohol derivative, acetic acid, 4-oxopentanoic acid, 4-methyl-4-hepten-3-one, propionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985
Humic acid, sodium salt	3 g of Na-huminate were heated at 700 °C for about 1 h in an air flow of 1.5 L/min	not applicable	CO ₂ , water, carboxylic acids, aliphatic hydrocarbons, phenols, coronene, anthraquinone, B[a]P, fluoranthene, perylene, B[a]P 27 µg/100 g salt, 1,2,5,6-dibenzanthracene 2 µg/100 g, 20-methylcholanthrene 2 µg/100 g, 2,3-benzofluoranthene 2 µg/100 g	Kröller, 1963c
<i>p</i> -Hydroxybenzoic acid ethylester (PHB ester)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH:</i> 1,2,5,6-dibenzanthracene, coronene, B[a]P 40 µg/100 g, fluoranthene, pyrene, 1,2,5,7-tetrahydropyrene, anthracene <i>Quinones:</i> anthraquinone <i>Phenols:</i> catechol, <i>p</i> -benzylphenol, <i>p</i> -sec-butylphenol <i>Others:</i> aliphatic hydrocarbons, benzoic acid, hydroxybenzoic acid, carbonyls	Kröller, 1970
Hydroxyethyl cellulose	30 g (in 0.5 g portions) of the cellulose derivate were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH:</i> tribenzopyrene, naphthacene, B[a]P 34 µg/100 g, fluoranthene, anthracene <i>Quinones:</i> anthraquinone <i>Phenols:</i> <i>m</i> -cresol, gallic acid, guajacol <i>Others:</i> acetic acid, formaldehyde, water, aliphatic hydrocarbons	Kröller, 1964a
Isoeugenol	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g): phenol 305, <i>o</i> -cresol 415, <i>m</i> -, <i>p</i> -cresol 1450	Schlotzhauer <i>et al.</i> , 1967
Isoprene (as Diels-Alder adduct with maleic anhydride)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	isoprene 37%	dipentene 2%	Robb <i>et al.</i> , 1964
Isoprene (as Diels-Alder adduct with cinnamaldehyde)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	isoprene 18% cinnamaldehyde 13%	benzene 2%, toluene 1%, styrene ca. 0.1%, dipentene ca. 0.1%, 2-phenyl-4-methylbenzaldehyde ca. 0.01%	Robb <i>et al.</i> , 1964
Lactic acid (sodium salt)	50 g (in 0.5 portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH:</i> fluoranthene, B[a]P 6 µg/100 g, 4,5-methylenephenanthrene, coronene <i>Quinones:</i> none <i>Phenols:</i> <i>o</i> -cresol <i>Others:</i> aliphatic hydrocarbons, formaldehyde, CO, CO ₂ , water	Kröller, 1966b
Lactose	Pyrolysis of lactose at 200–500 °C (reported here are only results obtained at 450–500 °C)	n.d.	<i>Composition of gases:</i> carbon dioxide 6.66%, carbon monoxide 35.08%, C _n H _{2n} 0.85%, methane 49.30%, hydrogen 7.56%	Tomasik, 1989
Lettuce leaves (from <i>Lactuca virosa</i>)	30 g (in 2 g portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	not applicable	<i>PAH:</i> B[a]P 5 µg/100 g, fluoranthene, phenanthrene <i>Quinones:</i> none <i>Phenols:</i> <i>p</i> -cresol, pyrogallol <i>Others:</i> aliphatic hydrocarbons, carboxylic acids, carbonyls	Kröller, 1970

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Licorice	Thermogravimetry/GC-MS ambient to 900 °C at 20 °C/min	not applicable	Decomposition, weight loss (%): 37–138 °C: 8% 138–380 °C: 44% 382–529 °C: 42% About 60 degraded compounds: acids, aldehydes, esters, ethers, hydrocarbons, ketones, alcohols, hydrocarbons, N-containing compounds	Chung and Aldridge, 1999 (A)
Licorice	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : 1,2,5,6-dibenzanthracene, 1,2-dihydropyrene, <i>p</i> -terphenyl, 20-methylcholanthrene, B[a]P 3 µg/100 g <i>Quinones</i> : anthraquinone <i>Phenols</i> : cresol, (pyrogallol) <i>Others</i> : aliphatic hydrocarbons, carboxylic acids, (furfural)	Kröller, 1967
Licorice	Dichloromethane extract of licorice was water suspended and steam distilled	n.d.	Most abundant volatile components were: acetol, propionic acid, 2-acetylpyrrole, 2-acetylfuran, furfuryl alcohol	Frattini <i>et al.</i> , 1977
Lignin (from wood)	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g): phenol 61, <i>o</i> -cresol 30, <i>m</i> -, <i>p</i> -cresol 114	Schlotzhauer <i>et al.</i> , 1967
Lignin	5–10 mg lignin were heated for 10 s at 700 °C under an N ₂ -flow (15 mL/min)	n.d.	<i>m</i> -, <i>p</i> -cresol 16.6%, phenol + <i>o</i> -cresol 12.3%, 4-ethylphenol 2.6%, 2-hydroxy-3-methyl-2-cyclopenten-1-one 1.8%, 2-ethyl-5-methylphenol 1.3%, 1,4-dimethoxybenzene 1.3%	Schlotzhauer <i>et al.</i> , 1985
Lignin	5 g of material was rapidly heated to 650 °C in a stream of nitrogen for 1 h	n.d.	<i>PAHs</i> (out of 11 investigated): pyrene 33 µg/100 g, B[a]P: 47 µg/100 g	Gilbert and Lindsey, 1957
Lignin	25 g material were pyrolysed at 800 °C in the following way: 12 cycles consisting of an “operative time” (20 s in a gas flow of nitrogen and air [1 L/min for each gas], simulating a puff) followed by an “inoperative time” (40 s in a flow of nitrogen, simulating the puff interval)	n.d.	<i>Major pyrolysis products (catechols)</i> : catechol 9.5 mg/g, guaiacol 5.2 mg/g, 4-methylcatechol 4.3 mg/g, phenol 2.3 mg/g, isoeugenol 1.1 mg/g	Schlotzhauer <i>et al.</i> , 1982
Madder lake (from <i>Rubia tinctorum</i>), major component: 1,2-dioxyanthraquinone	3 g of madder lake were heated at 700 °C for 1 h in an air flow of 1.5 L/min	not applicable	anthracene, fluoranthene, 1,4-dioxyanthraquinone, anthraquinone (as intermediate), B[a]P 12 µg/100 g	Kröller, 1963d
Malic acid	30 g (in 0.5 g portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : B[a]P 3 µg/100 g, fluoranthene, 20-methylcholanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : phenol, <i>m</i> -cresol <i>Others</i> : aliphatic hydrocarbons, carboxylic acids, CO, CO ₂ , water	Kröller, 1966b
Malic acid	5 g of material was rapidly heated at 650 °C in a stream of nitrogen for 1 h	n.d.	<i>PAHs</i> (out of 11 investigated): pyrene: 166 µg/100 g B[a]P: 35 µg/100 g	Gilbert and Lindsey, 1957
Melamine-formaldehyde resin	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : B[a]P 3 µg/100 g, fluoranthene, 2-methylphenanthrene <i>Quinones</i> : none <i>Phenols</i> : phenol, <i>o</i> -cresol <i>Others</i> : carbonyls, carboxylic acids, aliphatic hydrocarbons, (pyridines, ammonia)	Kröller, 1968
Melilot (from <i>Melilotus officinalis</i>)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : coronene, B[a]P 2 µg/100 g, anthracene, fluoranthene, 4,5-methylenephenanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>o</i> -cresol, catechol, pyrogallol <i>Others</i> : aliphatic hydrocarbons, carboxylic acids, aldehydes	Kröller, 1967
Menthol	1 g was pyrolysed for 5 min at 200–700 °C	200–500 °C: no degradation 500–700 °C: >98% unchanged	n.d.	Van Duuren <i>et al.</i> , 1968

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Menthol	Menthol was pyrolysed in a stream of nitrogen (30 mL/min) at 600 and 860 °C	78% in neutral fraction at 600 °C, which is 9 times as much menthol compared to 860 °C	Selected pyrolysis products (600/860 °C): phenol 29/192 mg/100 g benzene 11.9/17.5% styrene —/12.0% naphthalene —/3.7%	Schmeltz and Schlotzhauer, 1968
Methofuran (as Diels-Alder adduct with maleic anhydride)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	methofuran 30%	n.d.	Robb <i>et al.</i> , 1964
Methyl cellulose	30 g (in portions) of the cellulose derivate were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : picene, B[a]P 18 µg/100 g, fluoranthene, anthracene, 9,10- or 7,12-dimethyl-1,2-benzoanthracene <i>Quinones</i> : phenanthrenequinone, anthraquinone <i>Phenols</i> : <i>m</i> -cresol, pyrogallol <i>Others</i> : aliphatic hydrocarbons, acetic acid, formaldehyde, water, CO ₂	Kröller, 1964a
Methyl starch	30 g (in 0.5 g portions) of the additive were heated at 700 °C for up to 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : picene, B[a]P 16 µg/100 g, fluoranthene, anthracene <i>Quinones</i> : phenanthrenequinone, toluolquinone, anthraquinone <i>Phenols</i> : phenol, <i>m</i> -cresol, pyrogallol <i>Others</i> : aliphatic hydrocarbons, formaldehyde, acetic acid, formic acid, water	Kröller, 1966a
Monoacetin	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : coronene, B[a]P 6 µg/100 g, fluoranthene, anthracene <i>Quinones</i> : anthraquinone, phenanthrenequinone <i>Phenols</i> : phenol, <i>o</i> -ethylphenol, pyrogallol <i>Others</i> : glycerol, acetic acid, acetaldehyde, aliphatic hydrocarbons, CO ₂ , water	Kröller, 1968
Myrcene (as Diels-Alder adduct with maleic acid)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	myrcene 32%	n.d.	Robb <i>et al.</i> , 1964
Pectin	<i>Condition 1</i> : air, 100 mL/min 314 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 3</i> : air, 100 mL/min 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 4</i> : N ₂ , 100 mL/min 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	not applicable	Condition 1: 0.026% phenol Condition 3: 0.017% phenol Condition 4: 0.039% phenol	Bell <i>et al.</i> , 1966
Pectin (citrus)	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g): phenol 12, <i>o</i> -cresol 6, <i>m</i> -, <i>p</i> -cresol 8	Schlotzhauer <i>et al.</i> , 1967
Pectin	5 g of material was rapidly heated at 650 °C in a stream of nitrogen for 1 h	n.d.	<i>PAHs</i> (out of 11 investigated): pyrene 133 µg/100 g, B[a]P 45 µg/100 g	Gilbert and Lindsey, 1957
Pectin	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products</i> : acetic anhydride, acetoin, methyl formate, 3-methylfuran, 2-methyl-2-cyclopenten-1-one, furfural, acetylacetone, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, isomaltol, 2-furanmethanol, methyl-3-furanecarboxylate, cyclooctane, 3-methyl-2-hydroxycyclopentenone, hydroxyfuranone isomer, phenol, benzyl alcohol derivative, 4-oxopentanoic acid, furanecarboxylic acid derivative, 4-methyl-4-hepten-3-one, acetic acid, propionic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Peppermint leaves (from <i>Mentha piperita</i> L.)	30 g (in 2 g portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : B[a]P 5 µg/100 g, fluoranthene, pyrene, anthracene, 2-methyl-phenanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : phenol, β-naphthol, <i>m</i> -cresol <i>Others</i> : menthol, aliphatic hydrocarbons, carboxylic acids	Kröller, 1970
α-Phellandrene (as Diels-Alder adduct with maleic anhydride)	Adduct mixed with 3 times its weight of Celite and pyrolysed 1 min at 750 °C in a stream of nitrogen (15–25 mL/min)	α-phellandrene 8%	n.d.	Robb <i>et al.</i> , 1964
Polyethyleneglycol 400	30 g (in portions) of the humectant on silica were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	49% distillate with condensed and monoglycols	<i>PAH</i> : tribenzopyrene, pentacene, fluoranthene, 2,3-benzofluorene, B[a]P 10.5 µg/100 g, anthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : none <i>Others</i> : olefinic and aliphatic hydrocarbons, CO, CO ₂ , water, carboxylic acid(s), aldehyde(s)	Kröller, 1965a
Polyethyleneglycol 600	30 g (in portions) of the humectant on silica were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	22% distillate with triethylene glycol and other glycols	<i>PAH</i> : pentacene, B[a]P 29 µg/100 g, coronene, fluoranthene <i>Quinones</i> : anthraquinone, 2 unidentified <i>Phenols</i> : none <i>Others</i> : aldehyde(s), aliphatic hydrocarbons, water, carboxylic acid(s)	Kröller, 1965a
Polyethyleneglycol 1000	30 g (in portions) of the humectant on silica were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	16% distillate with triethylene glycol and other glycols	<i>PAH</i> : fluoranthene, anthracene, pentacene, coronene, B[a]P 42 µg/100 g <i>Quinones</i> : anthraquinone <i>Phenols</i> : polyphenol(s) <i>Others</i> : aldehyde(s), water, aliphatic hydrocarbons, carboxylic acid(s)	Kröller, 1965a
Polygalacturonic acid	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	not applicable	Formation of phenols (mg/100 g): phenol 14, <i>o</i> -cresol 7, <i>m</i> -, <i>p</i> -cresol 8	Schlotzhauer <i>et al.</i> , 1967
Potassium sorbate	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	(present)	<i>PAH</i> : coronene, B[e]P, fluoranthene, B[a]P 14 µg/100 g, phenanthrene, anthracene, acenaphthene <i>Quinones</i> : anthraquinone, phenanthrenequinone <i>Phenols</i> : β-naphthol, <i>o</i> -cresol, <i>o</i> -ethylphenol <i>Others</i> : aliphatic hydrocarbons, K ₂ CO ₃ (residue), carboxylic acids, aldehydes	Kröller, 1970
Proline	About 1 g of material was heated at 840 ± 10 °C in a stream of nitrogen (60 mL/min)	n.d.	<i>Selected pyrolysis products</i> : benzene 2.8%, indole 36.6%, pyridine 10.1%, quinone 2.0%, phenol 19.6%	Higman, E.B. <i>et al.</i> , 1970
Proline	Pyrolysis of 0.5–2.0 g at 800–860 °C in an N ₂ -flow	not applicable	<i>Principle products</i> : pyridine, isoquinoline, pyrrole, toluene, indole <i>Other products</i> : 2-methylpyridine, 3-/4-methylpyridine, aniline, quinoline, benzene, benzonitrile, <i>o</i> -tolunitrile, <i>m</i> -tolunitrile	Schmeltz <i>et al.</i> , 1972
Propylene glycol	Pyrolysis of 100 g of the polyalcohol was investigated at various temperatures	not applicable	<i>Principal compounds at 600 °C</i> : acetaldehyde 10–15 g/100 g acetone	Doihara <i>et al.</i> , 1964
1,2-Propylene glycol	2 mL of the glycol on silica were heated at 700 °C for about 10 min (until the glycol has disappeared) in an air flow of 1.5 L/min	50%	<i>PAH</i> : tribenzopyrene, coronene, fluoranthene, phenanthrene, B[a]P 6 µg/100 g <i>Quinones</i> : pyrenequinone, anthraquinone <i>Phenols</i> : none <i>Others</i> : aldehydes	Kröller, 1964b
<i>o</i> - <i>n</i> -Propylphenol	Pyrolysis at 700 °C in an N ₂ -flow (30 mL/min)	n.d.	Formation of phenols (mg/100 g): phenol 1600, <i>o</i> -cresol 13400, <i>m</i> -, <i>p</i> -cresol —	Schlotzhauer <i>et al.</i> , 1967
Prune extract	50 g (in portions) of the dried extract were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : B[a]P 3 µg/100 g, phenanthrene, fluoranthene, 20-methylcholanthrene <i>Quinones</i> : none <i>Phenols</i> : pyrogallol <i>Others</i> : aliphatic hydrocarbons, furfural, acetic acid, (aldehydes)	Kröller, 1967

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Rose leaves	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : 1,2,5,6-dibenzanthracene, B[a]P 2 µg/100 g, fluoranthene, anthracene, 7,12- or 9,10-dimethyl-1,2-benzanthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : phenol, <i>p</i> -cresol, β-naphthol, pyro-gallol <i>Others</i> : aliphatic hydrocarbons, carboxylic acids, aldehydes	Kröller, 1967
Rutin	<i>Condition 1: air, 100 mL/min</i> 314 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 3: air, 100 mL/min</i> 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 4: N₂, 100 mL/min</i> 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	n.d.	<i>Condition 1</i> : 0.008% phenol <i>Condition 3</i> : 0.004% phenol <i>Condition 4</i> : 0.028% phenol	Bell <i>et al.</i> , 1966
Rutin (trihydrate)	25 g material were pyrolysed at 800 °C in the following way: 12 cycles consisting of an "operative time" (20 s in a gas flow of nitrogen and air [1 L/min for each gas], simulating a puff) followed by an "inoperative time" (40 s in a flow of nitrogen, simulating the puff interval)	n.d.	<i>Major pyrolysis products (catechols)</i> : catechol: 7.8 mg/g 4-methylcatechol: 5.5 mg/g 4-ethylcatechol: 4.6 mg/g 4-propylcatechol: 1.2 mg/g	Schlotzhauer <i>et al.</i> , 1982
Shellac (resin excreted by <i>Lakshadia indica</i>)	30 g (in portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : pentacene, coronene, 1,2,5,6-dibenzanthracene, B[a]P 28 µg/100 g, fluoranthene, phenanthrene, anthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>o</i> -cresol, pyrogallol <i>Others</i> : acetic acid, aliphatic hydrocarbons, water	Kröller, 1966d
Sodium glycerophosphate	30 g (in portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : B[a]P 3 µg/100 g, fluoranthene, anthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : phenol <i>Others</i> : formaldehyde, aliphatic hydrocarbons, water	Kröller, 1966d
Sorbitol	30 g (in portions) of the humectant were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : tribenzopyrene, coronene, B[a]P 13 µg/100 g, fluoranthene, 4,5-methylenepheneanthrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>m</i> -cresol <i>Others</i> : formaldehyde, acetic acid, aliphatic hydrocarbons, water	Kröller, 1966d
Starch	<i>Condition 1: air, 100 mL/min</i> 314 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 3: air, 100 mL/min</i> 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) <i>Condition 4: N₂, 100 mL/min</i> 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	not applicable	<i>Condition 1</i> : 0.002% phenol <i>Condition 3</i> : 0.030% phenol <i>Condition 4</i> : 0.10% phenol	Bell <i>et al.</i> , 1966
Starch	30 g (in 0.5 g portions) of the additive were heated at 700 °C for about 10 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : picene, B[a]P 7 µg/100 g, fluoranthene, anthracene, 4,5-methylenepheneanthrene <i>Quinones</i> : phenanthrenequinone, anthraquinone <i>Phenols</i> : pyrogallol, gallic acid, <i>m</i> -cresol <i>Others</i> : aliphatic and olefinic hydrocarbons, water, furfural, acetic acid (formaldehyde)	Kröller, 1966a

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Starch	5 g of material was rapidly heated to 650 °C in a stream of nitrogen for 1 h	n.d.	PAHs (out of 11 investigated): pyrene 35 µg/100 g, B[a]P 17 µg/100 g	Gilbert and Lindsey, 1957
Sucrose (invert sugar, e.g. honey)	30 g (in portions) of the sugar were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	PAH: fluoranthene, anthracene, B[a]P 1 µg/100 g Quinones: anthraquinone Phenols: phenol Others: aliphatic hydrocarbons, furfural, carboxylic acids	Kröller, 1967
Sucrose	Condition 1: air, 100 mL/min 314 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace) Condition 3: air, 100 mL/min 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) Condition 4: N ₂ , 100 mL/min 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	n.d.	Condition 1: 0.067% phenol Condition 3: 0.062% phenol Condition 4: 0.082% phenol	Bell <i>et al.</i> , 1966
Sucrose	5–10 mg sucrose were heated for 10 s at 700 °C under an N ₂ -flow (15 mL/min)	n.d.	2-furaldehyde 67.1%, 5-methyl-2-furaldehyde 4.2%, 3-methylfuran 3.0%, 2-furanmethanol 2.4%, furancarboxylic acid methyl ester 2.0%, 1,3-cyclopentanedione 1.6%	Schlotzhauer <i>et al.</i> , 1985
Sucrose	Pyrolysis of sucrose at 200–500 °C (reported here are only results obtained at 450–500 °C)	n.d.	Composition of gases: CO ₂ 6.08%, CO 36.15%, C _n H _{2n} 0.73%, CH ₄ 47.40%, H ₂ 9.64%	Tomasik, 1989
Sucrose	5 g of material was rapidly heated at 650 °C in a stream of nitrogen for 1 h	n.d.	PAHs (out of 11 investigated): pyrene: 24 µg/100 g, B[a]P: 10 µg/100 g	Gilbert and Lindsey, 1957
Sucrose	200 g of sucrose (in 10–20 g portions) were heated with a gas burner under atmospheric pressure until evolution of aerosol ceased	n.d.	7.8% of volatile products Major products: 5-hydroxymethylfurfural and furfural	Gilbert and Lindsey, 1957
Sucrose	25 g material were pyrolysed at 800 °C in the following way: 12 cycles consisting of an "operative time" (20 s in a gas flow of nitrogen and air [1 L/min for each gas], simulating a puff) followed by an "inoperative time" (40 s in a flow of nitrogen, simulating the puff interval)	n.d.	Major pyrolysis products (catechols): furfural 27.7 mg/g, 5-hydroxymethylfurfural 19.5 mg/g	Schlotzhauer <i>et al.</i> , 1982
Sucrose	5 mg sucrose were heated for 10 s at 350–850 °C under an N ₂ -flow (15 mL/min)	n.d.	Formation of 5-hydroxymethylfurfural: 350 °C: 60.0 µg/mg sucrose 450 °C: 82.9 µg/mg sucrose 550 °C: 76.0 µg/mg sucrose 650 °C: 65.9 µg/mg sucrose 750 °C: 47.4 µg/mg sucrose 850 °C: 37.3 µg/mg sucrose	Schlotzhauer <i>et al.</i> , 1986
Sucrose ester (with 3-methylvaleric acid)	5 mg sucrose ester was heated for 10 s at 250–850 °C under an N ₂ -flow (15 mL/min)	n.d.	Temperature-dependent formation of: 3-methylvaleric acid: 60.7–67.3% 3-methylbutyric acid: 11.2–12.7% 5-hydroxy-methylfurfural: 8.9–14.6% 2-methylbutyric acid: 5.8–7.2% 4-methylvaleric acid: 1.3–2.6% isobutyric acid: 0.6–1.6%	Schlotzhauer <i>et al.</i> , 1986
Tartric acid (disodium salt)	50 g (in 0.5 portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	n.d.	PAH: B[e]P, B[a]P 4 µg/100 g, fluoranthene, 20-methylcholanthrene Quinones: anthraquinone Phenols: phenol, o-cresol Others: aliphatic hydrocarbons, aldehyde(s), pyruvic acid, CO, CO ₂ , water	Kröller, 1966b

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Tetracosane	Condition 3: air, 100 mL/min 777 °C (furnace 1) 562 °C (furnace 2) 685 °C (mobile furnace) Condition 4: N ₂ , 100 mL/min 315 °C (furnace 1) 320 °C (furnace 2) 685 °C (mobile furnace)	n.d.	Condition 3: 0.024% phenol Condition 4: 0% phenol	Bell <i>et al.</i> , 1966
Thiabendazole (2-(4'-thiazolyl)- benzimidazole)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	75%	<i>PAH</i> : anthracene, B[a]P < 1 µg/100 g, fluoranthene <i>Quinones</i> : none <i>Phenols</i> : none <i>Others</i> : thiophene, mercaptanes, H ₂ S, sulfur	Kröller, 1968
Tonka bean powder	5.7 g (in 1 g portions) were pyrolysed at 840 ± 10 °C under nitrogen	not applicable	<i>Neutrals</i> (0.22 g): benzene 14.1%, toluene 9.5%, styrene 15.9%, benzofuran 9.7%, indene 3.0%, naphthalene 13.7%, methylnaphthalene 3.2%, coumarin/acenaphthene 2.1%, phenanthrene/anthracene 4.5%, methylphenanthrene/anthracene 1.3% <i>Nitrogen bases</i> (0.03 g): pyridine 13.4%, picoline 4.3%, dimethylpyridine 3.2%, vinylpyridine 4.4%, indole 1.0%, quinoline 9.5%, isoquinoline 2.5%, methylquinoline 5.5%, carbazole 1.2%, benzoquinoline 2.9%, methylbenzoquinoline 1.6% <i>Phenols</i> (0.04 g): phenol 14.5%, cresol 8.1%, xlenol 1.1%, coumarin 2.3%, naphthol 9.2%	Higman <i>et al.</i> , 1974
Tragacanth	30 g (in 0.5–1.0 g portions) of the additive were heated at 700 °C for about 30 min (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : pentacene, coronene, B[a]P 23 µg/100 g, fluoranthene, anthracene, 20-methylcholanthrene <i>Quinones</i> : anthraquinone, phenanthrenequinone <i>Phenols</i> : phenol, o-cresol, carvacrol, (pyrogallol) <i>Others</i> : aliphatic hydrocarbons, water, formic acid, acetic acid	Kröller, 1965b
Tragacanth	10–15 mg of the additive were pyrolysed at 600 °C for 20 s (ramp 10 °C/ms)	not applicable	<i>Volatile pyrolytic products</i> : acetic anhydride, acetoin, methyl formate, 3-methylfuran, 2-methyl-2-cyclopenten- 1-one, furfural, acetylacetone, 2-furylmethylketone, 2,4-hexadienal, 5-methyl-2-furfural, isomaltol, 2-furanmethanol, cyclooctane, hydroxyfuranone isomer, benzyl alcohol derivative, 3-methyl-2- hydroxycyclopentenone, methyl-3- furanecarboxylate, phenol, 4-oxopentanoic acid, propionic acid, furanecarboxylic acid derivative, 4-methyl-4-hepten-3-one, acetic acid, 2-methylpropionic acid, butyric acid, 3-methylbutyric acid, pentanoic acid, hexanoic acid, octanoic acid, nonanoic acid, decanoic acid	Sjöberg and Pyysalo, 1985
Triacetin	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	(present)	<i>PAH</i> : B[a]P 4 µg/100 g, fluoranthene, anthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : phenol <i>Others</i> : acetic acid, glycerol, aliphatic hydrocarbons	Kröller, 1968
Triethylene glycol	2 mL of the glycol on silica were heated at 700 °C for about 10 min (until the glycol has disappeared) in an air flow of 1.5 L/min	80%	<i>PAH</i> : fluoranthene, 2,3-benzofluorene B[a]P ~ 15 µg/100 g, tribenzopyrene <i>Quinones</i> : anthraquinone <i>Phenols</i> : none <i>Others</i> : aldehydes	Kröller, 1964b

Table 5 (contd.)

Ingredient(s)	Pyrolysis conditions	Transfer (%)	Pyrolysis products	Reference(s)
Triglycerol	30 g (in portions) of the humectant were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	n.d.	<i>PAH</i> : 4,5-methylenephenanthrene, tribenzopyrene, fluoranthene, pentacene, coronene, anthracene <i>B[a]P</i> 10 µg/100 g <i>Quinones</i> : anthraquinone, phenanthrenequinone <i>Phenols</i> : phenol, <i>o</i> -ethylphenol, pyrogallol <i>Others</i> : glycerol 15%, acetaldehyde, acetic acid, aliphatic hydrocarbons, CO ₂ , water	Kröller, 1966d
Vanilla extract	17.8 g (in 5 g portions) were pyrolysed at 840 ± 10 °C under nitrogen	not applicable	<i>Neutrals</i> (0.28 g): benzene 12.3%, toluene 11.6%, furfural 5.5%, styrene 6.6%, benzofuran 4.8%, indene 6.2%, naphthalene 8.1%, methylnaphthalene 3.8%, acenaphthylene 2.3%, phenanthrene/anthracene 1.7%, methylphenanthrene/anthracene 1.6% <i>Nitrogen bases</i> (0.12 g): pyridine 18.8%, picoline 8.0%, dimethylpyridine 5.7%, vinylpyridine 5.6%, quinoline 2.8%, methylquinoline 0.6% <i>Phenols</i> (0.39 g): phenol 39.1%, cresol 26.5%, xylol 4.8%	Higman, H.C. et al., 1974
Vanilla roots (from <i>Trilisa odoratissima</i>)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : 2,3-benzofluorene, B[a]P 3 µg/100 g, fluoranthene, 1,2-dihdropyrene, <i>p</i> -terphenyl <i>Quinones</i> : anthraquinone <i>Phenols</i> : pyrogallol, phenol, <i>o</i> -cresol, ethylphenol <i>Others</i> : coumarine, carboxylic acids, aliphatic hydrocarbons, aldehydes	Kröller, 1967
Woodruff (from <i>Asperula odorata</i>)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	coumarin (present)	<i>PAH</i> : tribenzopyrene, fluoranthene, B[a]P 4 µg/100 g, phenanthrene, <i>p</i> -terphenyl <i>Quinones</i> : anthraquinone, phenanthrenequinone <i>Phenols</i> : catechol, pyrogallol <i>Others</i> : aliphatic hydrocarbons, carboxylic acids, aldehydes	Kröller, 1967
Yellow wood extract (from <i>Morus tinctoria</i>)	30 g (in 1 g portions) of the additive were heated at 700 °C (until the organic material has disappeared) in an air flow of 1.5 L/min	not applicable	<i>PAH</i> : fluoranthene, anthracene, 9,10-dihydroanthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : <i>o</i> - and <i>m</i> -cresol, pyrogallol, catechol <i>Others</i> : acetic acid, olefinic hydrocarbons, CO, CO ₂ , water	Kröller, 1966c
Yellow wood extract (in a mixture with diethylene glycol)	30 g (in portions) of the additive were heated at 700 °C until the organic material has disappeared in an air flow of 1.5 L/min	Glycol (present)	<i>PAH</i> : B[a]P 1 µg/100 g, fluoranthene, 4,5 methylenephenanthrene, anthracene <i>Quinones</i> : anthraquinone <i>Phenols</i> : pyrogallol, catechol <i>Others</i> : formaldehyde, acetic acid, aliphatic hydrocarbons	Kröller, 1968

Table 6. Biological activity of ingredients used on cigarette tobacco

Ingredient(s)	Experimental design	Biological effect/biological assay	Reference(s)
2 Ingredients: 1-octanol 1-decanol (M 58)	CSC of cigarettes $\pm$ 480 ppm alcohol mixture	→ Tumorigenicity in the mouse skin painting assay	Tso, 1975 (P)
2 Ingredients: glycerol propylene glycol (M 59)	MSS of cigarettes $\pm$ glycerol/propylene glycol, which were added in different combinations and concentrations; the mixtures used contained 12000/7000, 24000/14000 or 72000/42000 ppm glycerol/propylene glycol	→ Respiratory tract changes in a 13-week nose-only smoke inhalation study in Fischer 344 rats	Gaworski <i>et al.</i> , 1999b (A)
150 Flavor ingredients in 4 unique combinations (M 60)	Cigarette smoke condensate of cigarettes treated with 150 flavour ingredients (exaggerated concentrations if possible) in 4 unique flavour combinations vs. reference cigarettes without additives	→ Tumor promotion in a two stage mouse skin painting assay with SENCAR mice	Gaworski <i>et al.</i> , 1999a
172 Ingredients in 4 typical mixtures (M 61)	Mainstream smoke of cigarettes containing 172 ingredients in 4 typical mixtures (exaggerated concentrations if possible) vs. reference cigarettes without additives	→ Biological effects in a 13-week nose-only smoke inhalation study using Fischer 344 rats	Gaworski <i>et al.</i> , 1998
333 Ingredients in 3 different groups (M 62: Ingredient Group 1, M 63: Ingredient Group 2, M 64: Ingredient Group 3)	MSS and CSC of cigarettes $\pm$ 333 ingredients in 3 groups typically found in commercial cigarettes	→ Overall toxicity of cigarette smoke in the following biological assays: Ames Assay (according to OECD guideline 471), Neutral Red Assay (with BALB/c 3T3 cells), subchronic inhalation in Sprague-Dawley rats (according to OECD guideline 413) and chemical analysis of smoke composition and determination of risk indices	Carmines, 2002 ^a
Cellulose	CSC of cigarettes $\pm$ 10% cellulose	→ Tumorigenicity in the mouse skin painting assay with female ICR Swiss mice	NCI, Report No. 4, 1980
	Tobacco smoke of cigarettes $\pm$ 10% cellulose	→ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
Citric acid	Tobacco smoke of experimental cigarettes $\pm$ 1.25% citric acid	→ Ciliostasis in the trachea of cats exposed <i>in vivo</i> to the smoke of treated and control cigarettes	Dalhamn and Rylander, 1971
Cocoa	CSC of cigarettes $\pm$ 1% cocoa	↗ Tumorigenicity in the mouse skin painting assay with female ICR Swiss mice	NCI, Report No. 3, 1977
		↗ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
Cocoa	Tobacco smoke of cigarettes $\pm$ 1% cocoa	→ Particle clearance	
Cocoa	CSC of cigarettes $\pm$ 1 or 3% cocoa	→ Tumorous and non-tumorous lesions in the mouse skin painting assay with female ICR Swiss mice	Römer and Hackenberg, 1990
Diammonium phosphate	Tobacco smoke of different cigarettes (tobacco, reconstituted leaf tobacco and a mixture of both) $\pm$ DAP (3000–14200 ppm)	→ Histopathologic lesions, decreases in body weight gain, increases in blood COHb and serum nicotine and cotinine in a 13-week sub-chronic inhalation study in Fischer-344 rats	Misra <i>et al.</i> , 2001
Glycerol	MSS of cigarettes $\pm$ 72000 ppm glycerol	→ Respiratory tract changes in a 13-week nose-only smoke inhalation study in Fischer 344 rats	Gaworski <i>et al.</i> , 1999b (A)
Glycerol	CSC of cigarettes $\pm$ 2.8% glycerol	→ Tumorigenicity in the mouse skin painting assay with female ICR Swiss mice	NCI, Report No. 3, 1977
		↘ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
	Tobacco smoke of cigarettes $\pm$ 2.8% glycerol	↘ Chicken tracheal assay measuring particle clearance	
Menthol	Tobacco smoke of experimental cigarettes $\pm$ menthol	→ Ciliostasis using human, rabbit or rat respiratory epithelium in <i>in vitro</i> experiments	Rakieten <i>et al.</i> , 1952

Table 6 (contd.)

Ingredient(s)	Experimental design	Biological effect/biological assay	Reference(s)
Menthol	Mainstream smoke (MSS) of cigarettes $\pm$ synthetic <i>l</i> -menthol [5000 ppm (<i>w/w</i>)]	→ Toxicity in a 13-week nose-only smoke inhalation study using Fischer 344 rats	Gaworski <i>et al.</i> , 1997
Menthol	Mainstream smoke CSC of different cigarettes (Eclipse and an ultralight brand)	→ <i>In vitro</i> toxicology test batterie including sister chromatide exchanges and neutral red cytotoxicity in CHO cells and the Ames assay	Bombick <i>et al.</i> , 2001
Propylene glycol	MSS of cigarettes $\pm$ 42000 ppm propylene glycol	→ Respiratory tract changes in a 13-week nose-only smoke inhalation study in Fischer 344 rats	Gaworski <i>et al.</i> , 1999b (A)
Sugar	CSC of cigarettes $\pm$ 5.3% invert sugar	→ Tumorigenicity in mouse skin painting assay with female ICR Swiss mice → cytotoxicity in a growth inhibition assay using the human KB tumor cell line → ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	NCI, Report No. 3, 1977
Sugar	CSC of high and low-“tar” cigarettes + different sugars (glucose, fructose, galactose, sorbitol, sucrose, lactose in concentrations from 0.2 to 1.18 g/cig) vs. reference cigarettes without the addition of sugar	→ Mutagenicity in the Ames assay using strains TA98 and TA 100 with metabolic activation (no reduction without metabolic activation); the lowest mutagenicities were 37% (high-“tar” cigarettes) and 22% (low-“tar” cigarettes) in comparison to control cigarettes without addition of sugars	Sato <i>et al.</i> , 1979

^aCarmines, 2002: stands on behalf of the following series of publications: Carmines, 2002; Römer *et al.*, 2002; Rustemeier *et al.*, 2002 and Vanscheeuwijck *et al.*, 2002.

Table 7. Biological activity of experimental ingredients

Ingredient(s)	Experimental design	Biological effect/biological assay	Reference(s)
3 Ingredients: titanyl chloride sodium hydroxide wood pulp (M 39)	CSC of experimental cigarettes $\pm$ 7% titanyl chloride, sodium hydroxide (for pH adjustment to pH 5.5) and 7.5% wood pulp	➤ Tumorigenicity in skin painting assays using female Swiss ICR mice ➔ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line: no ranking possible	NCI, Report No. 1, 1976
	Tobacco smoke of experimental cigarettes $\pm$ 7% titanyl chloride and sodium hydroxide (for pH adjustment to pH 5.5) and 7.5% wood pulp	➔ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance ➤ Biological activity using an <i>in vitro</i> macrophages inhibition assay	
3 Ingredients: ethylhydroxyethyl cellulose methocel sulfite pulp (M 40)	CSC of experimental cigarettes $\pm$ a mixture of 1.84% ethylhydroxyethyl cellulose 7.35% methocel and 4.59% refined, unbleached sulfite pulp	➤ Tumorigenicity in skin painting assays using female Swiss ICR mice ➔ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line: no ranking possible	NCI, Report No. 1, 1976
	Tobacco smoke of experimental cigarettes $\pm$ a mixture of 1.84% ethylhydroxyethyl cellulose 7.35% methocel and 4.59% refined, unbleached sulfite pulp	➤ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance ➤ Biological activity using an <i>in vitro</i> macrophages inhibition assay	
2 Ingredients: magnesium nitrate zinc oxide (M 45)	CSC of cigarettes $\pm$ 5.61% magnesium nitrate and 6.96% zinc oxide	➤ Tumorigenicity in the mouse skin painting assay with female ICR Swiss mice ➤ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line	NCI, Report No. 3, 1977
	Tobacco smoke of cigarettes $\pm$ 5.61% magnesium nitrate and 6.96% zinc oxide	➤ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
4 Ingredients: cellulose ether gums dialdehyde cross-linker galacto-mannan gums sulfite pulp (M 46)	CSC of experimental cigarettes $\pm$ a mixture of 0.52% cellulose ether gums 0.58% dialdehyde crosslinker 5.85% galacto-mannan gums and 6.05% refined unbleached sulfite pulp	➤ Tumorigenicity in skin painting assays in female ICR Swiss mice ➔ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line	NCI, Report No. 4, 1980
	Tobacco smoke of experimental cigarettes $\pm$ a mixture of 0.52% cellulose ether gums 0.58% dialdehyde crosslinker 5.85% galacto-mannan gums and 6.05% refined unbleached sulfite pulp	➔ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
6 Ingredients in a mixture: cellulose ether gums dialdehyde cross-linker galacto-mannan gums sulfite pulp sodium hydroxide citric acid (M 47)	CSC of experimental cigarettes $\pm$ a mixture of 0.52% cellulose ether gums 0.58% dialdehyde crosslinker 5.85% galacto-mannan gums 6.05% refined, unbleached sulfite pulp 3.2% sodium hydroxide and 2.8% citric acid	➤ Tumorigenicity in skin painting assays using female ICR Swiss mice ➔ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line	NCI, Report No. 4, 1980
	Tobacco smoke of experimental cigarettes $\pm$ a mixture of 0.52% cellulose ether gums 0.58% dialdehyde crosslinker 5.85% galacto-mannan gums 6.05% refined, unbleached sulfite pulp 3.2% sodium hydroxide and 2.8% citric acid	➔ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
Chemosol (M 65)	CSC of cigarettes with and without "Chemosol" (citric acid and deuterium oxide in distilled water)	➔ Tumorigenicity in mouse skin painting assays with Swiss ICR mice	Gargus <i>et al.</i> , 1975
Aluminium oxide	CSC of experimental cigarettes $\pm$ aluminium oxide (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Aluminium oxide (activated)	CSC of experimental cigarettes $\pm$ aluminium oxide (activated) (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Aluminium oxide (aerated)	CSC of experimental cigarettes $\pm$ aluminium oxide (aerated, 4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Aluminium oxide trihydrate	CSC of experimental cigarettes $\pm$ aluminium oxide trihydrate (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961

Table 7 (contd.)

Ingredient(s)	Experimental design	Biological effect/biological assay	Reference(s)
Aluminium oxide trihydrate	CSC of experimental cigarettes $\pm$ aluminium trihydrate $\times 3 \text{ H}_2\text{O}$	➤ Tumorigenicity in mouse skin painting assays	Hoffmann and Wynder, 1968
Aluminium silicate	CSC of experimental cigarettes $\pm$ aluminium silicate (1 and 4%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Ammonium sulfamate	CSC of cigarettes with ammonium sulfamate (5, 6 and 7.5 mg/cig) treated paper in comparison to untreated control cigarettes	➔ No statistically significant differences in final tumor incidence, but significantly lower tumor incidence during earlier test periods in mouse skin painting assays with female ICR Swiss mice was caused by the addition of ammonium sulfamate	Bock <i>et al.</i> , 1974
Boric acid	CSC of experimental cigarettes $\pm$ boric acid (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Calcium carbonate	CSC of experimental cigarettes $\pm$ calcium carbonate (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Cobalt (III) oxide	CSC of experimental cigarettes $\pm$ cobalt (III) oxide (4–5%)	➔ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Copper nitrate	CSC of experimental cigarettes $\pm$ 5% copper nitrate	➤ Tumorigenicity in mouse skin painting assays	Hoffmann and Wynder, 1968
Copper nitrate	CSC of experimental cigarettes $\pm$ copper (II) nitrate (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Copper nitrate	CSC of experimental cigarettes $\pm$ 5% copper nitrate	➤ Tumor multiplicity in mouse skin painting assays using HA/ICR/Mil (Swiss Albino) female mice	Wynder and Hoffmann, 1969
Diethylamine citrate	Tobacco smoke of experimental cigarettes $\pm$ 3.12% diethylamine citrate	➔ Ciliostasis in the trachea of cats exposed <i>in vivo</i> to the smoke of treated cigarettes	Dalhamn and Rylander, 1971
Magnesium nitrate	CSC of experimental cigarettes $\pm$ 10% magnesium nitrate	➤ Mutagenicity in Ames test strains TA 1538 liver and lung S9 mix and TA 1535 $\pm$ liver S9 mix; ➔ no activity could be measured using the frameshift mutant strains TA 1536 and TA 1537	Kier <i>et al.</i> , 1974
Magnesium nitrate	CSC of cigarettes $\pm$ 5.72% magnesium nitrate	➤ Tumorigenicity in the mouse skin painting assay with female ICR Swiss mice	NCI, Report No.3, 1977
Magnesium nitrate	Tobacco smoke of cigarettes $\pm$ 5.72% magnesium nitrate	➤ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line ➔ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	
Magnesium oxide	CSC of experimental cigarettes $\pm$ magnesium oxide (4–5%)	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Wynder and Hoffmann, 1961
Methyl caprate	CSC of cigarettes $\pm$ 480 ppm methyl caprate	➔ Tumorigenicity in the mouse skin painting assay	Tso, 1975 (P)
Nickel acetate	CSC of experimental cigarettes $\pm$ nickel acetate	➤ Tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Hoffmann and Wynder, 1968
Nitrate	CSC of experimental cigarettes $\pm$ nitrate (total nitrate content from 0.22–0.59%)	➤ Tumorigenicity in mouse skin painting assays when the amount of total nitrate is greater than about 0.4%	Collins <i>et al.</i> , 1981
Nitrate	CSC of experimental cigarettes containing 1.8% nitrate vs. untreated reference cigarettes (nitrate was adjusted to 1.8% in experimental cigarettes)	➤ Tumorigenicity in mouse skin painting assays using female CFP mice (genetically identical with ICI mice) for about 5–10% (application of 33 and 66 mg condensate per painting)	Dontenwill <i>et al.</i> , 1976
Oxolamine citrate	Tobacco smoke of experimental cigarettes $\pm$ 5% oxolamine citrate	➤ Ciliostasis in the trachea of cats exposed <i>in vivo</i> to the smoke of treated cigarettes	Dalhamn, 1969
Palladium	CSC of experimental cigarettes $\pm$ palladium (total palladium content from 0–580 ppm)	➤ Tumorigenicity in mouse skin painting assays when the amount of non-extractable palladium is greater than about 100 ppm	Collins <i>et al.</i> , 1981
Phenylmethyl-oxadiazole (PMO)	Tobacco smoke of experimental cigarettes $\pm$ 0.5–10% phenylmethyloxadiazole	➤ Ciliostasis in the trachea of cats exposed <i>in vivo</i> to the smoke of cigarettes containing 2% PMO	Dalhamn and Rylander, 1971

Table 7 (contd.)

Ingredient(s)	Experimental design	Biological effect/biological assay	Reference(s)
Phenylmethyl-oxadiazole (PMO)	Tobacco smoke of experimental cigarettes $\pm$ 2% phenylmethyloxadiazole	➤ Inhibition of pulmonary particle clearance (mucus transport and phagocytic activity of the lung) using guinea pigs exposed to smoke and to a mixed aerosol of killed radioactive and viable <i>Escherichia coli</i> bacteria (complete protection)	Rylander, 1971
Phenylmethyl-oxadiazole (PMO)	Tobacco smoke of experimental cigarettes $\pm$ 2% phenylmethyloxadiazole	➤ Inhibition of pulmonary clearance in guinea pigs exposed to smoke and to a mixed aerosol of killed radioactive and viable <i>Escherichia coli</i> bacteria (complete protection) ➤ Increase in macrophages in long-term exposures in guinea pigs (complete protection) ➤ Irritation in respiratory epithelium of guinea pigs (partial protection)	Rylander, 1973
Phenylmethyl-oxadiazole (PMO)	Tobacco smoke of experimental cigarettes $\pm$ 2% phenylmethyloxadiazole	➔ Decrease in weight gain in Sprague-Dawley rats exposed to tobacco smoke (no protection) ➤ Increase in goblet cell count in the trachea of exposed Sprague-Dawley rats (complete protection) ➤ Increase in epithelial thickness and cell number in the trachea of exposed Sprague-Dawley rats (partial protection) ➤ Increasing number of cells in mitosis in the trachea, bronchial pathways, alveoli and oesophagus of Sprague-Dawley rats exposed to tobacco smoke (partial protection)	Jones <i>et al.</i> , 1972
Phenylmethyl-oxadiazole (PMO)	Tobacco smoke of experimental cigarettes $\pm$ 2% phenylmethyloxadiazole	➤ Increase in goblet cell number in the tracheal epithelium of exposed Sprague-Dawley rats ➔ Shift from neutral to acid glycoproteins within goblet cells and increase in secretory mass within goblet cells in exposed Sprague-Dawley rats ➤ Increase in cell size in the tracheal gland and increase in the thickness of the gland in exposed Sprague-Dawley rats	Jones <i>et al.</i> , 1973
Phenylvinylloxadiazole	Tobacco smoke of experimental cigarettes $\pm$ 2.02% phenylvinylloxadiazole	➤ Ciliostasis in the trachea of cats exposed <i>in vivo</i> to the smoke of treated cigarettes	Dalhamn and Rylander, 1971
Potassium nitrate	CSC of experimental cigarettes containing 2.2% nitrate (partially added as potassium nitrate) in comparison to control cigarettes with 1.1% nitrate	➔ Tumorigenicity in skin painting assays using female Swiss ICR mice ➔ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line: no ranking possible	NCI, Report No.1, 1976
	Tobacco smoke of experimental cigarettes containing 2.2% nitrate (partially added as potassium nitrate) in comparison to control cigarettes with 1.1% nitrate	➤ Ciliotoxicity using an <i>in vitro</i> chicken tracheal assay measuring particle clearance ➔ Ciliotoxicity using an <i>in vivo</i> chicken tracheal assay measuring particle clearance ➤ Biological activity using an <i>in vitro</i> macrophages inhibition assay	
Potassium nitrate	CSC of reconstituted tobacco (RT) $\pm$ 5% potassium nitrate in comparison to normal tobacco	➔ Only slight differences in tumor promotion in mouse skin painting assays were found comparing RT with and without potassium nitrate; RT ($\pm$ potassium nitrate) led to a significant reduction of the tumorigenicity (39% of the biological activity of natural tobacco)	Halter and Ito, 1972
Potassium nitrate	CSC of reconstituted tobacco (RT) $\pm$ potassium nitrate in comparison to cigarettes made from original tobacco	➤ CSC of RT caused a decrease in tumorigenicity for more than 50% and addition of 5% KNO₃ to RT caused a slight reduction of tumorigenicity in mouse skin painting assays using female Swiss ICR mice	Hoffmann and Wynder, 1972
Potassium nitrate	CSC of experimental cigarettes $\pm$ 3% potassium nitrate ₃	➤ Toxicity and tumorigenicity in mouse skin painting assays with female Swiss ICR mice	Hoffmann and Wynder, 1968
Sodium nitrate	CSC of experimental cigarettes soaked in 10 ⁻² M sodium nitrate was prepared smoking the cigarettes in the presence of vapors of HNO ₃ or acetic acid to enable the development of nitroarenes	➤ Direct acting mutagenicity in the Ames test (strains TA 98, TA 98NR and TA 98/1,8-DNP₃ were used) which was reduced by about 70% using a strain deficient in the "classical" nitro-reductase (TA 98NR)	McCoy and Rosenkranz, 1982
Sodium nitrate	CSC of experimental cigarettes $\pm$ 8.3% sodium nitrate	➤ Toxicity and tumorigenicity in mouse skin painting assays with female Swiss ICR mice	Hoffmann and Wynder, 1968

Table 7 (contd.)

Ingredient(s)	Experimental design	Biological effect/biological assay	Reference(s)
Sodium nitrate	CSC of experimental cigarettes + 8% sodium nitrate vs. untreated reference cigarettes	↘ Laryngeal tumorigenicity in long-term inhalation studies using Syrian Golden hamsters; leucoplakia was reduced for about 50% and early invasive carcinomas were reduced for about 75%	Dontenwill, 1974
Sodium nitrate	CSC of experimental cigarettes with different tobacco mixtures ± 8.3% sodium nitrate	↘ Toxicity and tumorigenicity in mouse skin painting assays with female Ha/ICR/Mil (Swiss Albino) mice	Hoffmann and Wynder, 1967
Sodium nitrate	CSC of experimental cigarettes ± 8.3% sodium nitrate	↘ Tumor multiplicity in mouse skin painting assays using HA/ICR/Mil (Swiss Albino) female mice	Wynder and Hoffmann, 1969
Sodium nitrate	CSC of experimental cigarettes with different tobacco mixtures ± 8% sodium nitrate	↘ Tumorigenicity in mouse skin painting assay with female ICI mice	Dontenwill <i>et al.</i> , 1972
Zinc oxide	CSC of cigarettes ± 7.09% zinc oxide	→ Tumorigenicity the mouse skin painting assay with female ICR Swiss mice ↘ Cytotoxicity in a growth inhibition assay using the human KB tumor cell line	NCI, Report No.3, 1977
	Tobacco smoke of cigarettes ± 7.09% zinc oxide	↘ Ciliotoxicity using an <i>in vitro</i> and <i>in vivo</i> chicken tracheal assay measuring particle clearance	