

Raw materials for the manufacture of quaternary ammonium compounds, betaines and amine oxides

# Composition

Dimethyl fatty alkylamines

## **Marketed grades**

Genamin CC 302 D	Genamin 8/10 R 302 D
Genamin CS 302 D	Genamin 12 R 302 D
Genamin LA 302 D	Genamin 14 R 302 D
Genamin MY 302 D	Genamin 16 R 302 D
Genamin SH 302 D	Genamin 18 R 302 D
Genamin TA 302 D	Genamin 20/22 R 302 D

The code letters of numbers followed by "R" in the product designation indicate the nature of the alkyl radical. The code letters "SH" and "CS" stand for alkyl radicals with the chainlength distribution of stearic or a special coconut fatty acid. Numbers followed by "R" indicate the chainlength of the alkyl radical. The chainlength distribution of individual products can be seen from table 1.

The number 302 common to all alkyl dimethylamines represents the tertiary nitrogen with 2 methyl groups; the code letter "D" indicates that the product is a distilled grade.

The most important physical and chemical data of the distilled Genamin 302 grades are summarized in table 1. Technical grades and amines with other alkyl radicals can be supplied on request.

Dimethyl fatty alkylamines are valuable raw materials for the manufacture of surfactants. These waterinsoluble tertiary amines can be readily converted to water-soluble salts, quaternary ammonium compounds, often referred to simply as "quats", are the most important. Like cationic surfactants generally, they have substantivity for most materials, e.g. glass and cotton. This property is utilized in many different industries, e.g. the textile, petroleum and polish industries. Closely allied to this substantivity are the excellent disinfectant and preservative properties of these compounds.

# **Properties**

Dimethyl fatty alkylamines are liquid or pasty, waterinsoluble bases. They are readily soluble in organic solvents such as mineral oil, isopropanol and chloroform. The basicity of the dimethyl fatty amines is slightly less marked than that of primary and secondary fatty amines

## Safety precautions

Fatty amines are strong organic bases. Therefore special care must be taken when working with these products.

Please see detailed safety precautions in the MSDS of each dimethyl fatty alkylamine.

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# Reactions

Like primary and secondary amines, dimethyl fatty alkylamines form salts with organic and inorganic acids:

$$R = N \xrightarrow{CH_3}_{CH_3} + HCI \xrightarrow{CH_3}_{R = N \xrightarrow{CH_3}_{H_3}} R = N \xrightarrow{CH_3}_{H_3} + R'COOH \xrightarrow{CH_3}_{R = N \xrightarrow{H_3}_{H_3}} R = N \xrightarrow{CH_3}_{H_3} R'COO^- (2)$$

The salts of inorganic and short-chain organic acids are readily water-soluble; those of long-chain organic acids are soluble primarily in organic solvents.

Dimethyl fatty alkylamines react with alkylation agents to produce the versatile quaternary ammonium compounds.

$$R = N \begin{pmatrix} CH_3 \\ CH_3 \end{pmatrix} + CH_3CI \longrightarrow R = N \begin{pmatrix} CH_3 \\ I_+ \\ R = N \end{pmatrix} CH_3 \qquad (3)$$

$$R = N \begin{pmatrix} CH_3 \\ CH_3 \end{pmatrix} + C_6H_5CH_2CI \longrightarrow R = N - CH_2 - C_6H_5 \quad CI^- \qquad (4)$$

$$R = N \xrightarrow{CH_3} + (CH_3O)_2SO_2 \xrightarrow{} R = N \xrightarrow{CH_3} CH_3OSO_3^- (5)$$

The betaines which are of interest in cosmetics manufacture, can be obtained by reaction with ahalogen carboxylic acid salts.

$$R = N \begin{pmatrix} CH_3 \\ CH_3 \end{pmatrix} + CICH_2COONa \xrightarrow[-NaCl]{I_1} R = N \begin{pmatrix} CH_3 \\ I_4 \\ -CH_2 - COO \end{pmatrix} (6)$$

Other recations which are easy to carry out are conversion with hydrogen peroxide to the corresponding amine oxides and with ethylene oxide to quaternary ethoxy ammonium salts:

$$R = N \xrightarrow{CH_3} + H_2O_2 \xrightarrow{CH_3} R = N \xrightarrow{CH_3} O + H_2O$$
(7)

$$\begin{array}{c} \mathsf{CH}_{3} \\ \mathsf{R}-\mathsf{N}_{-}^{+}\mathsf{H} \\ \mathsf{CI}_{-}^{-}+\mathsf{CH}_{2}^{-}\cdot\mathsf{CH}_{2} \end{array} \xrightarrow{\mathsf{CH}_{3}} \mathsf{R}-\mathsf{N}_{-}^{+}\mathsf{CH}_{2}\mathsf{CH}_{2}\mathsf{O}\mathsf{H} \\ \mathsf{CI}_{3} \\ \mathsf{CH}_{3} \end{array} \xrightarrow{\mathsf{CH}_{3}} \mathsf{R}-\mathsf{N}_{-}^{+}\mathsf{CH}_{2}\mathsf{C}\mathsf{H}_{2}\mathsf{O}\mathsf{H} \\ \mathsf{CI}_{3} \end{array} \xrightarrow{\mathsf{CH}_{3}} (8)$$

# Uses of dimethyl fatty alkylamine derivatives

#### Quaternary ammonium compounds

The quaternary ammonium compounds which are accessible by reactions 3, 4, 5 and 8 have a wide range of uses, of which only the most important are mentioned here:

#### Disinfectants

Quaternary fatty ammonium salts are compounds with a strong bactericidal and fungicidal action. A typical example is coconut alkyldimethylbenzyl ammonium chloride. An important outlet for these compounds is in disinfectant cleaners for industrial and domestic use. They have also achieved considerable importance in human and veterinary medicine.

They are also used for controlling algae, for instance in cooling water and swimming baths.

#### **Cosmetics**

Quaternary ammonium compounds are widely used especially in the formulation of hair care products. They move substantively on to the hair and thus improve its appearance, handle and combing properties.

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#### Textile industry

Quaternary ammonium compounds are used in the textile industry as softeners, re-wetting and antistatic and antibacterial finishing agents. Quaternary compounds have proved to be successful levelling agents and retarders in acrylic fibre dyeing.

#### Other uses

Quaternary ammonium compounds also serve as acid inhibitors, emulsifiers, dispersing agents, vulcanization accelerators, antistatic agents and auxillaries in paint application by electrodeposition processes.

#### Betaines

The betaines which can be produced from dimethyl fatty alkylamines according to reaction 6 in acid solution act as cationic surfactants and in alkaline solution as inner neutral salts:

$$\begin{array}{c} CH_{3} \\ I \\ R - N - CH_{2} - COO^{-} \\ I \\ CH_{3} \end{array} \xrightarrow{+ HX} \qquad \begin{array}{c} CH_{3} \\ I \\ -HX \end{array} \qquad \begin{array}{c} R - N - CH_{2} - COOH \\ CH_{2} - COOH \end{array} X^{-} \qquad (9)$$

Despite the quaternary N atom present in the molecule, betaines can be employed together with surface-active anions; this characteristic is utilized especially in cosmetics.

#### **Amine Oxides**

The amine oxides which are readily derived from dimethyl fatty alkylamines (reaction 7) are very important. These compounds are good surfactants and, unlike fatty alkyl ammonium salts, can be used together with anionic compounds without impairment of their surface-active properties. Amine oxides are used especially in the following fields:

#### Detergent industry

Here they serve primarily as foam stabilizers, in liquid acid and alkaline toilet cleaners, solubilizing agents and skin protective components in washing-up liquids and carpet shampoos.

#### **Cosmetics**

In cosmetic preparations amine oxides function as foam stabilizers and emulsifiers.

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Table 1.0

## **Product properties** \*)

	Genamin CC 302 D	Genamin CS 302 D	Genamin LA 302 D	Genamin MY 302 D	Genamin SH 302 D	Genamin TA 302 D
Chemical composition	Dimethyl coconut	Dimethyl coconut	Dimethyl lauryl	Dimethyl myristyl	Dimethyl stearyl	Dimethyl tallow
	fatty amine, dist.	fatty amine, dist.	amine, dist.	amine, dist.	amine, dist.	fatty amine, dist.
Appearance (20 °C)	liquid	liquid	liquid	liquid	liquid	liquid
Amine value [mg KOH/g] DIN 16945	233 - 255	230 - 250	244 - 255	227 - 239	184 - 199	186 - 198
Molar mass [g/mol]	220 - 240	225 - 244	220 - 230	235 - 247	282 – 305	283 - 301
Tertiary amine content [equiv%]	min. 99	min. 99	min. 99	min. 99	min. 99	min. 98
Approx. mean chain						
distribution [%]						
C8	2 – 6					
C10	4 – 8	max. 3	max. 1.5	max. 5		
C12	48 – 56	52 – 62	64 – 73	36 – 43		max. 1.5
C14	15 – 21	20 – 26	22 – 29	45 – 53	8	2 – 6
C <sub>16</sub>	7 – 13	9 – 13	2 – 6	8 – 12	25 – 37	23 – 37
C18	7 – 13	5 – 9	max. 1.5		58 – 70	55 – 75
C <sub>20</sub>					max. 3	max. 2
C22						
Hazen colour	max. 50	max. 50	max. 50	max. 50	max. 80	max. 100
EN 1557						
lodine value	max. 1	max. 1	max. 1	max. 1	max. 1	35 - 50
[g J2/100 g]						
Pour point [° C]	-10	-10	< -10	- 10	15	5
DIN/ISO 3016						
Flash point [° C]	130	130	130	140	165	160
DIN/ISO 2592						
Density at 60 °C [g/cm <sup>3</sup> ]	0.77	0.77	0.77	0.77	0.78	0.78
DIN 51757						

\*) These characteristics are for guidance only and not to be taken as product specifications. The tolerances are given in the product specification sheet. For further product properties, specifications, safety and ecological data, please refer to the MSDS.

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	Genamin 8/10 R 302 D	Genamin 12 R 302 D	Genamin 14 R 302 D	Genamin 16 R 302 D	Genamin 18 R 302 D	Genamin 20/22 R 302 D
Chemical composition	Dimethyl octyl-/	Dimethyl dodecyl	Dimethyl tetradecyl	Dimethyl hexadecyl	Dimethyl octadecyl	Dimethyl eicosyl-/
	decylamine, dist.	amine, dist.	amine, dist.	amine, dist.	amine, dist.	docosyl amine, dist.
Appearance (20 °C)	liquid	liquid	liquid	liquid	liquid up to pasty	pasty, wax-like
Amine value [mg KOH/g] DIN 16945	303 -331	247 - 260	221 - 235	198 - 209	175 - 187	155 - 165
Molar mass [g/mol]	170 - 185	216 - 227	238 - 254	268 - 283	300 - 320	340 - 362
Tertiary amine content [equiv%]	min. 99	min. 99	min. 99	min. 99	min. 99	min. 99
Approx. mean chain distribution [%] C6 C8 C10 C12 C14 C14 C16 C18 C20 C22 C22 C24 Hazen colour	max. 1 37 – 50 49 – 61 max. 3.5 max. 50	min. 95 max. 50	min. 95 max. 50	max. 5 min. 94 max. 4 max. 50	max. 5 min. 92 max. 2 max. 50	max. 1.4 max. 7 11 - 16 75 - 81 max. 1 max. 50
EN 1557	may 1	may 1	may 1	may 1	mov. 1	mov. 1
[g J2/100 g]	max. T	max. I	max. I	max. I	max. T	max. I
Pour point [° C] DIN/ISO 3016	< -15	< -15	0	10	20	27 - 33
Flash point [° C] DIN/ISO 2592	> 100	> 100	> 100	> 150	> 150	> 150
Density at 60 °C [g/cm <sup>3</sup> ] DIN 51757	0.77	0.77	0.77	0.78	0.78	0.79

### Table 1.1**Product properties**\*)

\*) These characteristics are for guidance only and not to be taken as product specifications. The tolerances are given in the product specification sheet. For further product properties, specifications, safety and ecological data, please refer to the MSDS.

This information is based on our present state of knowledge and is intended to provide general notes on our products and their uses. It should not therefore be construed as guaranteeing specific properties of the products described on their suitability for a particular application. Any existing industrial property rights must be observed. The quality of our products is guaranteed under our General Conditions of Sale.

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