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## How to identify a substance produced in different qualities

### Introduction

Fragrance AH consists of several isomers. It is produced in three different qualities (qualities X, Y and Z), which differ in the ratio of these isomers.

### Composition

The substance, consisting of five isomers (A, B, C, D and E), is manufactured with the following composition:

Constituents	Concentration ranges (%)			Overall range (%)
	Quality X	Quality Y	Quality Z	
<b>Isomer A:</b> 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	80 - 85	65 - 75	50 - 60	50 - 85
<b>Isomer B:</b> 3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	6 - 10	3 - 7	3 - 7	3 - 10
<b>Isomer C:</b> [R-(E)]-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	3 - 11	10 - 20	20 - 30	3 - 30
<b>Isomer D:</b> 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one	0.5 - 1.5	2 - 4	2 - 4	0.5 - 4
<b>Isomer E:</b> 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one	0.5 - 1.5	4 - 6	10 - 15	0.5 - 15

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## Identification

### Option 1: Separate registrations for each quality

Based on the 80/10 rule described in the [Guidance for identification and naming of substances under REACH and CLP](#), the three qualities have different names, as follows:

- Quality X contains one main constituent (Isomer A) with a concentration  $\geq 80$  %. It is therefore named as a mono-constituent substance:

3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one

- Quality Y contains two main constituents (Isomers A and C) with a concentration  $\geq 10$  % and  $< 80$  %. It is therefore named as a multi-constituent substance:

Reaction mass of 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one and [R-(E)]-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one

- Quality Z contains three main constituents (Isomers A, C and E) with a concentration  $\geq 10$  % and  $< 80$  %. It is therefore named as a multi-constituent substance:

Reaction mass of 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one and [R-(E)]-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one and 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one

### Option 2: A single registration for all qualities (justification required)

It is possible to identify the substance as a multi-constituent substance based on the constituents present at concentrations  $\geq 10$  % across all three qualities (see table for overall range concentration values). It will therefore be named as a reaction mass of four isomers (Isomers A, B, C, E), as follows:

Reaction mass of 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)but-3-en-2-one and 3-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)but-3-en-2-one and [R-(E)]-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one and 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one

However, a justification for this approach is required because of the deviation from the 80 % rule and the 10 % rule described in the [Guidance for identification and naming of substances under REACH and CLP](#).

The following issues need to be addressed in the justification:

- Available test data covers the variability of the three qualities;
- All qualities have very similar physico-chemical properties;
- All qualities have the same hazard classification and labelling; and
- All qualities are used in a similar way and have similar exposure scenarios (thus, similar chemical safety reports).