

*Horst Surburg*  
*Johannes Panten*

# **Common Fragrance and Flavor Materials**

Preparation, Properties and Uses

*6 completely revised and updated Edition*

**WILEY-VCH**  
Verlag GmbH & Co. KGaA

## Contents

<b>1</b>	<b>Introduction</b>	<i>1</i>
1.1	History	<i>1</i>
1.2	Definition	<i>2</i>
1.3	Physiological Importance	<i>2</i>
1.4	Natural, Nature-Identical, and Artificial Products	<i>3</i>
1.5	Sensory Properties and Chemical Structure	<i>3</i>
1.6	Volatility	<i>4</i>
1.7	Threshold Concentration	<i>4</i>
1.8	Sensory Properties	<i>4</i>
1.8.1	Fragrance Ingredients	<i>5</i>
1.8.2	Flavoring Substances	<i>6</i>
<b>2</b>	<b>Individual Fragrance and Flavor Materials</b>	<i>7</i>
2.1	Aliphatic Compounds	<i>8</i>
2.1.1	Hydrocarbons	<i>8</i>
2.1.1.1	( <i>E,Z</i> )-1,3,5-Undecatriene [51447-08-6]	<i>8</i>
2.1.1.2	1,3-Undecadien-5-yne [166432-52-6]	<i>9</i>
2.1.2	Alcohols	<i>9</i>
2.1.2.1	3-Octanol [589-98-0]	<i>9</i>
2.1.2.2	2,6-Dimethyl-2-heptanol [13254-34-7]	<i>10</i>
2.1.2.3	( <i>E</i> )-2-Hexen-1-ol [928-95-0]	<i>10</i>
2.1.2.4	( <i>Z</i> )-3-Hexen-1-ol [928-96-1], Leaf Alcohol	<i>10</i>
2.1.2.5	1-Octen-3-ol [3391-86-4]	<i>10</i>
2.1.2.6	9-Decen-1 (cipher)-ol [13019-22-2]	<i>11</i>
2.1.2.7	10-Undecen-1-ol [112-43-6]	<i>11</i>
2.1.2.8	3,4,5,6,6-Pentamethylheptan-2-ol [87118-95-4]	<i>11</i>
2.1.2.9	(2 <i>E</i> ,6 <i>Z</i> )-2,6-Nonadien-1-ol [28069-72-9], Violet Leaf Alcohol	<i>11</i>
2.1.2.10	4-Methyl-3-decen-5-ol [81782-77-6]	<i>12</i>
2.1.3	Aldehydes and Acetals	<i>12</i>
2.1.3.1	Hexanal [66-25-1], Caproaldehyde, Aldehyde C <sub>6</sub>	<i>13</i>
2.1.3.2	Octanal [124-13-0], Caprylaldehyde, Aldehyde C <sub>8</sub>	<i>13</i>
2.1.3.3	Nonanal [124-19-6], Pelargonaldehyde, Aldehyde C <sub>9</sub>	<i>13</i>

- 2.1.3.4 Decanal [112-31-2], Caprinaldehyde, Aldehyde C<sub>10</sub> 14
- 2.1.3.5 Undecanal [112-44-7], Aldehyde C<sub>11</sub> 14
- 2.1.3.6 Dodecanal [112-54-9], Lauraldehyde, Lauric Aldehyde, Aldehyde C<sub>12</sub> 14
- 2.1.3.7 Tridecanal [10486-19-8] 14
- 2.1.3.8 2-Methyldecanal [19009-56-4], Methyloctylacetaldehyde, Aldehyde MOA 14
- 2.1.3.9 2-Methylundecanal [110-41-8], Methylnonylacetaldehyde, Aldehyde MNA 15
- 2.1.3.10 (*E*)-2-Hexenal [6728-26-3], Leaf Aldehyde 16
- 2.1.3.11 (*Z*)-4-Heptenal [6728-31-0] 16
- 2.1.3.12 2,6-Dimethyl-5-hepten-1-al [106-72-9] 16
- 2.1.3.13 (*E*)-4-Decenal [65405-70-1] 16
- 2.1.3.14 10-Undecenal [112-45-8] 17
- 2.1.3.15 2-Dodecenal [20407-84-5] 17
- 2.1.3.16 2,6,10-Trimethyl-5,9-undecadienal [24048-13-3] and [54082-68-7] 17
- 2.1.3.17 1,1-Dimethoxy-2,2,5-trimethyl-4-hexene [67674-46-8] 17
- 2.1.4 Ketones 18
- 2.1.4.1 3-Hydroxy-2-butanone [52217-02-4], Acetoin 18
- 2.1.4.2 2,3-Butanedione [431-03-8], Diacetyl 18
- 2.1.4.3 (*2E*)-5-Methyl-2-hepten-4-one [81925-81-7] 18
- 2.1.4.4 3,4,5,6,6-Pentamethyl-3-hepten-2-one [81786-73-4] 19
- 2.1.4.5 2,4,4,7-Tetramethyl-6-octen-3-one [74338-72-0] 19
- 2.1.5 Acids and Esters 20
- 2.1.5.1 2-Methyl-2-pentenoic Acid [3142-72-1] 20
- 2.1.5.2 Ethyl Formate [109-94-4] 21
- 2.1.5.3 (*Z*)-3-Hexenyl Formate [33467-73-1] 21
- 2.1.5.4 Ethyl Acetate [141-78-6] 21
- 2.1.5.5 Butyl Acetate [123-86-4] 21
- 2.1.5.6 Isoamyl Acetate [123-92-2] 21
- 2.1.5.7 Hexyl Acetate [142-92-7] 21
- 2.1.5.8 3,5,5-Trimethylhexyl Acetate [58430-94-7], Isononyl Acetate 21
- 2.1.5.9 (*E*)-2-Hexenyl Acetate [2497-18-9] 22
- 2.1.5.10 (*Z*)-3-Hexenyl Acetate [3681-71-8] 22
- 2.1.5.11 Ethyl Propionate [105-37-3] 22
- 2.1.5.12 Ethyl Butyrate [105-54-4] 22
- 2.1.5.13 Butyl Butyrate [109-21-7] 22
- 2.1.5.14 Isoamyl Butyrate [106-27-4] 23
- 2.1.5.15 Hexyl Butyrate [2639-63-6] 23
- 2.1.5.16 (*Z*)-3-Hexenyl Isobutyrate [41519-23-7] 23
- 2.1.5.17 Ethyl Isovalerate [108-64-5] 23
- 2.1.5.18 Ethyl 2-Methylbutyrate [7452-79-1] 23
- 2.1.5.19 Ethyl Hexanoate [123-66-0], Ethyl Caproate 23
- 2.1.5.20 Ethyl 2-Methylpentanoate [39255-32-8] 24

- 2.1.5.21 2-Propenyl Hexanoate [123-68-2], Allyl Caproate 24
- 2.1.5.22 Ethyl Heptanoate [106-30-9], Ethyl Enanthate 24
- 2.1.5.23 2-Propenyl Heptanoate [142-19-8], Allyl Heptanoate, Allyl Enanthate 24
- 2.1.5.24 Ethyl Octanoate [106-32-1], Ethyl Caprylate 24
- 2.1.5.25 Methyl 2-Nonenoate [111-79-5] 24
- 2.1.5.26 Ethyl (2E,4Z)-2,4-Decadienoate [3025-30-7], Pear Ester 25
- 2.1.5.27 Methyl 2-Octynoate [111-12-6], Methyl Heptin Carbonate 25
- 2.1.5.28 Methyl 2-Nonynoate [111-80-8], Methyl Octin Carbonate 25
- 2.1.5.29 Propyl (2S)-2-(1,1-Dimethylpropoxy)propanoate [319002-92-1] 25
- 2.1.5.30 Ethyl 3-Oxobutanoate, Ethyl Acetoacetate [141-97-9] 25
- 2.1.5.31 (Z)-3-Hexenyl Methyl Carbonate [67633-96-9] 26
- 2.1.5.32 Allyl (3-Methylbutoxy)acetate, Isopentyloxyacetic Acid Allyl Ester [67634-00-8], [67634-01-9] Allyl Amylglycolate 26
- 2.1.6 Miscellaneous Compounds 26
- 2.1.6.1 Allyl Isothiocyanate [57-06-7], Allyl Mustard Oil 27
- 2.1.6.2 5-Methyl-3-heptanone oxime, N-Hydroxy-5-methyl-3-heptanimine [22457-23-4] 27
- 2.1.6.3 3-[(Z)-3-Hexenyloxy]-propanenitrile [142653-61-0] 27
- 2.1.6.4 N,2,3-Trimethyl-2-isopropylbutanamide [51115-67-4] "WS 23" 28
- 2.1.6.5 2-Tridecenitrile [22629-49-8] 28
- 2.2 Acyclic Terpenes 29
- 2.2.1 Hydrocarbons 29
- 2.2.2 Alcohols 29
- 2.2.2.1 Geraniol [106-24-1], (2E)-3,7-Dimethyl-2,6-octadien-1-ol 30
- 2.2.2.2 Nerol [106-25-2], (2Z)-3,7-Dimethyl-2,6-octadien-1-ol 32
- 2.2.2.3 Linalool [78-70-6], 3,7-Dimethyl-1,6-octadien-3-ol 32
- 2.2.2.4 Myrcenol [543-39-5], 2-Methyl-6-methylene-7-octen-2-ol 35
- 2.2.2.5 Citronellol [26489-01-0], 3,7-Dimethyl-6-octen-1-ol 36
- 2.2.2.6 Dihydromyrcenol [18479-58-8], 2,6-Dimethyl-7-octen-2-ol 37
- 2.2.2.7 Tetrahydrogeraniol [106-21-8], 3,7-Dimethyloctan-1-ol 38
- 2.2.2.8 Tetrahydrolinalool [78-69-3], 3,7-Dimethyloctan-3-ol 38
- 2.2.2.9 2,6-Dimethyl-2-octanol [18479-57-7], Tetrahydromyrcenol 39
- 2.2.2.10 7-Methoxy-3,7-dimethyl-2-octanol [41890-92-0] 39
- 2.2.2.11 Farnesol [4602-84-0], 3,7,11-Trimethyl-2,6,10-dodecatrien-1 (cipher)-ol 39
- 2.2.2.12 Nerolidol [7212-44-4], 3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol 40
- 2.2.3 Aldehydes and Acetals 41
- 2.2.3.1 Citral [5392-40-5], 3,7-Dimethyl-2,6-octadien-1-al 41
- 2.2.3.2 Citral Diethyl Acetal [7492-66-2],  
1,1-Diethoxy-3,7-dimethyl-2,6-octadiene 43
- 2.2.3.3 Citronellal [106-23-0], 3,7-Dimethyl-6-octen-1-al 43
- 2.2.3.4 7-Hydroxydihydrocitronellal [107-75-5], "Hydroxycitronellal,"  
3,7-Dimethyl-7-hydroxyoctan-1-al 44

- 2.2.3.5 Methoxydihydrocitronellal [3613-30-7],  
3,7-Dimethyl-7-methoxyoctan-1-ol 45
- 2.2.3.6 Hydroxydihydrocitronellal Dimethyl Acetal [141-92-4],  
8,8-Dimethoxy-2,6-dimethyloctan-2-ol 46
- 2.2.3.7 2,6,10-Trimethyl-9-undecenal [141-13-9] 46
- 2.2.4 Ketones 46
- 2.2.4.1 Geranylacetone [689-67-8],  
6,10-Dimethyl-5,9-undecadien-2-one 47
- 2.2.5 Acids and Esters 47
- 2.2.5.1 Geranyl and Neryl Esters 48
- 2.2.5.2 Linalyl Esters 49
- 2.2.5.3 Citronellyl and Dihydromyrcenyl Esters 50
- 2.2.6 Miscellaneous Compounds 51
- 2.2.6.1 3,7-Dimethyloctanenitrile [40188-41-8] 52
- 2.2.6.2 Citronellic Acid Nitrile [51566-62-2], Citronellyl Nitrile 52
- 2.3 Cyclic Terpenes 52
- 2.3.1 Hydrocarbons 52
- 2.3.1.1 Limonene [138-86-3], 1,8-*p*-Menthadiene 54
- 2.3.1.2  $\gamma$ -Terpinene [99-85-4], 1,4-*p*-Menthadiene 54
- 2.3.1.3 (-)- $\alpha$ -Phellandrene [4221-98-1], 1,5-*p*-Menthadiene 55
- 2.3.1.4  $\alpha$ -Pinene [80-56-8], 2-Pinene,  
2,6,6-Trimethylbicyclo[3.3.1]hept-2-ene 55
- 2.3.1.5  $\beta$ -Pinene [127-91-3], 2(10)-Pinene 56
- 2.3.2 Alcohols and Ethers 56
- 2.3.2.1 Menthol, *p*-Menthan-3-ol 56
- 2.3.2.2 Isopulegol, 8-*p*-Menthen-3-ol,  
5-Methyl-2-(1-methylethenyl)-cyclohexanol [7786-67-6],  
[50373-36-9] 61
- 2.3.2.3  $\alpha$ -Terpineol [98-55-5], 1-*p*-Menthen-8-ol 62
- 2.3.2.4 1-Terpinen-4-ol [562-74-3], 1-*p*-Menthen-4-ol 63
- 2.3.2.5 *cis*-4-(Isopropyl)cyclohexanemethanol, *cis*-Hexahydrocuminyll  
Alcohol [13828-37-0], *cis*-*p*-Menthan-7-ol 64
- 2.3.2.6 Borneol, *endo*-2-Bornanol [507-70-0] 64
- 2.3.2.7 3-[(*l*)-Menthoxyl]propane-1,2-diol [87061-04-9], (*l*)-Menthyl  
Glyceryl Ether 65
- 2.3.2.8 Cedryl Methyl Ether [19870-74-7] and [67874-81-1] 66
- 2.3.3 Aldehydes and Ketones 66
- 2.3.3.1 Menthone, *p*-Menthan-3-one [10458-14-7] 66
- 2.3.3.2 Carvone, 1,8-*p*-Menthadien-6-one 67
- 2.3.3.3 Camphor, 1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one [76-22-2] 69
- 2.3.3.4 Fenchone, 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one  
[1195-79-5] 69
- 2.3.3.5 Ionones and Homologous Compounds 69
- 2.3.3.6 Damascones, 1-(2,6,6-Trimethylcyclohexenyl)-2-buten-1-ones 74

- 2.3.3.7  $\alpha$ -Damascone, 1-(2,6,6-Trimethyl-2-cyclohexenyl)-2-buten-1-one [43052-87-5]; (Z)-: [23726-94-5]; (E)-: [24720-09-0] 74
- 2.3.3.8  $\beta$ -Damascone, 1-(2,6,6-Trimethyl-1-cyclohexenyl)-2-buten-1-one [35044-68-9]; (Z)-: [23726-92-3]; (E)-: [23726-91-2] 74
- 2.3.3.9  $\beta$ -Damasconone [23726-93-4],  
1-(2,6,6-Trimethyl-1,3-cyclohexadienyl)-2-buten-1-one 75
- 2.3.3.10  $\delta$ -Damascone, 1-(2,6,6-Trimethyl-3-cyclohexenyl)-2-buten-1-one [57378-68-4]; (E)-1 $\alpha$ ,2 $\beta$ : [71048-82-3] 75
- 2.3.3.11 1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one [39872-57-6] 75
- 2.3.3.12 1,3,4,6,7,8a-Hexahydro-1,1,5,5-tetramethyl-2H-2,4a-methanonaphthalen-8(5H)one [23787-90-8] 76
- 2.3.3.13 Nootkatone, 4,4a-Dimethyl-6-isopropenyl-4,4a,5,6,7,8-hexahydro-3H-naphthalen-2-one [4674-50-4] 76
- 2.3.3.14 Methyl Cedryl Ketone, "MCK," Acetyl Cedrene 76
- 2.3.4 Esters 77
- 2.3.4.1  $\alpha$ ,3,3-Trimethylcyclohexane-1-methanol Formate [25225-08-5] 77
- 2.3.4.2 (-)-Menthyl Acetate, (-)-*p*-Menthan-3-yl Acetate [2623-23-6] 78
- 2.3.4.3 *rac*-Menthyl Acetate [29066-34-0] 78
- 2.3.4.4 Menthanyl Acetate, Dihydroterpinyl Acetate [58985-18-5] 78
- 2.3.4.5 5-Methyl-2-(1-methylethyl)cyclohexyl 2-Hydroxy-propanoate [59259-38-0], *l*-Menthyl Lactate 79
- 2.3.4.6  $\alpha$ -Terpinyl Acetate [80-26-2], 1-*p*-Menthen-8-yl Acetate 79
- 2.3.4.7 Nopyl Acetate [35836-72-7],  
(-)-2-(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)-ethyl Acetate 80
- 2.3.4.8 Bornyl acetate, 2-*endo*-bornanyl Acetate [76-49-3] 80
- 2.3.4.9 Isobornyl Acetate [125-12-2], 2-*exo*-bornanyl Acetate 80
- 2.3.4.10 *N*-substituted *p*-Menthane-3-Carboxamides 81
- 2.3.4.11 *N*-ethyl-*p*-menthane-3-carboxamide [39711-79-0], "WS 3" (1) 81
- 2.3.4.12 *N*-(4-Methoxyphenyl)-*p*-menthane-3-carboxamide [68489-09-8] "WS 12" (2) 82
- 2.3.4.13 *N*-[[5-methyl-2-(1-methylethyl)cyclohexyl]carbonyl]glycine Ethyl Ester [68489-14-5] "WS 5" (3) 82
- 2.3.4.14 Methyl 2,2-dimethyl-6-methylene-1-cyclohexanecarboxylate [81752-87-6] 82
- 2.3.4.15 Ethyl 2,6,6-Trimethyl-1,3-cyclohexadiene-1-carboxylate [35044-59-8] 82
- 2.3.4.16 Guaiyl Acetate [94333-88-7] 83
- 2.3.4.17 Cedryl Acetate [77-54-3] 83
- 2.3.4.18 Vetiveryl Acetate [62563-80-8] 83
- 2.3.5 Miscellaneous Compounds 84
- 2.3.5.1 8-Mercapto-*p*-menthan-3-one [38462-22-5] 84
- 2.3.5.2 1-*p*-Menthene-8-thiol [71159-90-5] 85
- 2.4 Other Cycloaliphatic Compounds 85
- 2.4.1 Alcohols and Ethers 85

- 2.4.1.1 1-(4-Isopropylcyclohexyl)ethanol [63767-86-2] 85
- 2.4.1.2 4-Cyclohexyl-2-methyl-2-butanol [83926-73-2] 86
- 2.4.1.3 2-Methyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)butanol [72089-08-8] 86
- 2.4.1.4 2-Methyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol [28219-60-5] 87
- 2.4.1.5 5-(2,2,3-Trimethyl-3-cyclopenten-1-yl)-3-methylpentan-2-ol [65113-99-7] 87
- 2.4.1.6 2-Ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol [28219-61-6] 88
- 2.4.1.7 3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol [67801-20-1] 88
- 2.4.1.8 2-Methyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-pentenol [104864-90-6] 88
- 2.4.1.9 3,3-Dimethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol [107898-54-4] 89
- 2.4.1.10 [1-Methyl-2-(1,2,2-trimethyl[3.1.0]hex-3-ylmethyl)cyclopropyl]methanol [198404-98-7] 89
- 2.4.1.11 3-*trans*-Isocamphylcyclohexanol [4105-12-8] 89
- 2.4.1.12 1-(2,2,6-Trimethylcyclohexyl)hexan-3-ol [70788-30-6] 90
- 2.4.1.13 2,5,5-Trimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-ol [41199-19-3], Ambrinol 91
- 2.4.1.14 1-[[2-(1,1-Dimethylethyl)cyclohexyl]oxy]-2-butanol, [139504-68-0] 91
- 2.4.1.15 2-(2,2,7,7-Tetramethyltricyclo[6.2.1.0](1,6)undec-5-en-5-yl)propan-1-ol, 2-(2,2,7,7-Tetramethyltricyclo[6.2.1.0](1,6)undec-4-en-5-yl)propan-1-ol, [929625-08-1], [1001252-30-7] 92
- 2.4.1.16 Cyclododecyl Methyl Ether [2986-54-1], Methoxycyclododecane 92
- 2.4.1.17 (Ethoxymethoxy)cyclododecane [58567-11-6] 92
- 2.4.2 Aldehydes 93
- 2.4.2.1 2,4-Dimethyl-3-cyclohexene Carboxaldehyde [68039-49-6] 93
- 2.4.2.2 4-(4-Methyl-3-penten-1-yl)-3-cyclohexene Carboxaldehyde [37677-14-8] 93
- 2.4.2.3 1-Methyl-4-(4-methyl-3-penten-1-yl)-3-cyclohexene Carboxaldehyde [52474-60-9] 93
- 2.4.2.4 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene Carboxaldehyde [31906-04-4] 94
- 2.4.2.5 2-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-butenal [3155-71-3] 94
- 2.4.3 Ketones 94
- 2.4.3.1 2-Pentylcyclopentanone [4819-67-4] 94
- 2.4.3.2 2-Heptylcyclopentanone [137-03-1] 95
- 2.4.3.3 2,2,5-Trimethyl-5-pentylcyclopentanone [65443-14-3] 95

- 2.4.3.4 Dihydrojasmane[1128-08-1],  
3-Methyl-2-pentyl-2-cyclopenten-1-one 96
- 2.4.3.5 (Z)-Jasmone [488-10-8],  
3-Methyl-2-[(2Z)-2-penten-1-yl]-2-cyclopenten-1-one 96
- 2.4.3.6 4-*tert*-Pentylcyclohexanone [16587-71-6] 97
- 2.4.3.7 6,7-Dihydro-1,1,2,3,3-pentamethyl-4(5*H*)-indanone  
[33704-61-9] 97
- 2.4.3.8 Cyclopentadecanone [502-72-7] 97
- 2.4.3.9 (E/Z)-3-Methyl-5-cyclotetradecen-1-one [259854-70-1] 98
- 2.4.3.10 (Z)-4-Cyclopentadecenone [14595-54-1] 98
- 2.4.3.11 3-Methylcyclopentadecanone [541-91-3], Muscone 99
- 2.4.3.12 3-Methylcyclopentadecenone [82356-51-2] 99
- 2.4.3.13 Cyclohexadecanone [2550-52-9] 100
- 2.4.3.14 5-Cyclohexadecen-1-one [37609-25-9] 100
- 2.4.3.15 (E/Z)-7/8-Cyclohexadecenone (Mixture of Isomers) [888642-03-9],  
[3100-36-5] 101
- 2.4.3.16 (E/Z)-8-Cyclohexadecenone [3100-36-5] 101
- 2.4.3.17 (Z)-9-Cycloheptadecen-1-one [542-46-1], Civetone 102
- 2.4.3.18 1-(5,5-Dimethyl-1-cyclohexen-1-yl)-4-penten-1-one  
[56973-85-4] 102
- 2.4.3.19 2-Cyclohexyl-1,6-heptadien-3-one [313973-37-4] 102
- 2.4.3.20 1-Spiro[4.5]dec-7-en-7-yl-4-penten-1-one,  
1-Spiro[4.5]dec-6-en-7-yl-4-penten-1-one [224031-70-3] 103
- 2.4.3.21 2,3,8,8-Tetramethyl-1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl Methyl  
Ketone [54464-57-2], (1-1,2,3,4,5,6,7,8-Octahydro-2,3,8,8-  
tetramethyl-2-naphthyl)ethan-1-one [166090-45-5],  
OTNE 103
- 2.4.3.22 4-(2-Butenylidene)-3,5,5-trimethyl-2-cyclohexene-1-one and  
Isomers [13215-88-8] 104
- 2.4.3.23 Methyl 2,6,10-Trimethyl-2,5,9-cyclododecatrien-1-yl Ketone  
[28371-99-5] 104
- 2.4.3.24 2-Hydroxy-3-methyl-2-cyclopenten-1-one;  
3-Methyl-2-cyclopenten-2-ol-1-one [80-71-7], Cyclotene 105
- 2.4.3.25 4-(1-Ethoxyvinyl)-3,3,5,5-tetramethylcyclohexanone  
[36306-87-3] 105
- 2.4.4 Esters 106
- 2.4.4.1 2-*tert*-Butylcyclohexyl Acetate [88-41-5], OTBCHA 106
- 2.4.4.2 4-*tert*-Butylcyclohexyl Acetate [32210-23-4], PTBCHA 106
- 2.4.4.3 (Z)-3-Hexenyl Cyclopropanecarboxylate [188570-78-7] 107
- 2.4.4.4 4,7-Methano-3a,4,5,6,7,7a-hexahydro-5 (or 6)-Indenyl Acetate  
[2500-83-6] (or [5413-60-5]) 107
- 2.4.4.5 Allyl 3-Cyclohexylpropionate [2705-87-5] 107
- 2.4.4.6 Ethyl 2-Ethyl-6,6-dimethyl-2-cyclohexenecarboxylate [57934-97-1],  
and Ethyl 2,3,6,6-Tetramethyl-2-cyclohexenecarboxylate  
[77851-07-1] 108



- 2.4.4.7 Allyl Cyclohexyloxyacetate [68901-15-5], Cyclohexyloxyacetic Acid Allyl Ester 108
- 2.4.4.8 [2-[1-(3,3-Dimethylcyclohexyl)ethoxy]-2-methyl-propyl] Propanoate [141773-73-1] 108
- 2.4.4.9 [2-[1-(3,3-Dimethylcyclohexyl)ethoxy]-2-oxo-ethyl] Propanoate; 2-(1-Oxopropoxy)-acetic Acid 1-(3,3-Dimethylcyclohexyl)ethyl Ester [236391-76-7] 109
- 2.4.4.10 Methyl Jasmonate [1211-29-6], 3-Oxo-2-[(2Z)-2-pentenyl]cyclopentaneacetic Acid Methyl Ester 109
- 2.4.4.11 Methyl Dihydrojasmonate [24851-98-7], Methyl (3-oxo-2-pentyliclopentyl)acetate 110
- 2.4.4.12 Methyl 2-Hexyl-3-oxocyclopentanecarboxylate [37172-53-5] 112
- 2.4.5 Miscellaneous Compounds 113
- 2.4.5.1 1,5-Dimethylbicyclo[3.2.1]octan-8-one oxime [75147-23-8] 113
- 2.5 Aromatic Compounds 113
- 2.5.1 Hydrocarbons 113
- 2.5.2 Alcohols and Ethers 113
- 2.5.2.1 Benzyl Alcohol [100-51-6] 114
- 2.5.2.2 Phenylethyl Alcohol [60-12-8], 2-Phenylethyl Alcohol 115
- 2.5.2.3 Phenylethyl Methyl Ether [3558-60-9] 116
- 2.5.2.4 Phenylethyl Isoamyl Ether [56011-02-0] 116
- 2.5.2.5 Acetaldehyde Ethyl Phenylethyl Acetal [2556-10-7] 116
- 2.5.2.6 1-Phenylethyl Alcohol [98-85-1], Styrallyl Alcohol 116
- 2.5.2.7 Dihydrocinnamic Alcohol [122-97-4], 3-Phenylpropanol 117
- 2.5.2.8 2,2-Dimethyl-3-phenyl-1-propanol [13351-61-6] 117
- 2.5.2.9 2,2-Dimethyl-3-(3-methylphenyl)propanol [103694-68-4] 118
- 2.5.2.10  $\alpha,\alpha$ -Dimethylphenylethyl Alcohol [100-86-7], 2-Methyl-1-phenyl-2-propanol,  $\alpha,\alpha$ -Dimethyl Benzyl Carbinol 118
- 2.5.2.11 2-Methyl-4-phenyl-2-butanol [103-05-9],  $\alpha,\alpha$ -Dimethylphenylethyl Carbinol 118
- 2.5.2.12 2-Methyl-5-phenylpentanol [25634-93-9] 119
- 2.5.2.13 3-Methyl-5-phenylpentanol [55066-48-3] 119
- 2.5.2.14 3-Methyl-1-phenyl-3-pentanol [10415-87-9], Phenylethyl Methyl Ethyl Carbinol 119
- 2.5.2.15 Cinnamic alcohol [104-54-1], 3-Phenyl-2-propen-1-ol 120
- 2.5.3 Aldehydes and Acetals 120
- 2.5.3.1 Benzaldehyde [100-52-7] 121
- 2.5.3.2 Phenylacetaldehyde [122-78-1] 121
- 2.5.3.3 Phenylacetaldehyde Dimethyl Acetal [101-48-4] 122
- 2.5.3.4 Dihydrocinnamaldehyde [104-53-0], 3-Phenylpropanal 122
- 2.5.3.5 Hydratropaldehyde [93-53-8], 2-Phenylpropanal 122
- 2.5.3.6 Hydratropaldehyde Dimethyl Acetal [90-87-9] 123
- 2.5.3.7 4-Methylphenylacetaldehyde [104-09-6] 123
- 2.5.3.8 3-Methyl-5-phenylpentanal [55066-49-4] 123
- 2.5.3.9 3-(4-Ethylphenyl)-2,2-dimethylpropanal [67634-15-5] 123

- 2.5.3.10 3-[4-(1,1-Dimethylethyl)phenyl]propanal [18127-01-0] 124
- 2.5.3.11 Cyclamenaldehyde [103-95-7],  
2-Methyl-3-(4-isopropylphenyl)propanal 124
- 2.5.3.12 3-(3-Isopropylphenyl)butanal [125109-85-5] 125
- 2.5.3.13 4-*tert*-Butyl- $\alpha$ -methyl-dihydrocinnamaldehyde [80-54-6],  
2-Methyl-3-(4-*tert*-butyl-phenyl)propanal, BMHCA 125
- 2.5.3.14 2-Methyl-3-[4-(2-methylpropyl)phenyl]propanal [6658-48-6] 126
- 2.5.3.15 Cinnamaldehyde [14371-10-9], 3-Phenyl-2-propenal 126
- 2.5.3.16  $\alpha$ -Amylcinnamaldehyde [122-40-7],  
2-Pentyl-3-phenyl-2-propenal 127
- 2.5.3.17  $\alpha$ -Hexylcinnamaldehyde [101-86-0],  
2-Hexyl-3-phenyl-2-propenal 127
- 2.5.4 Ketones 128
- 2.5.4.1 Acetophenone [98-86-2], Methyl Phenyl Ketone 128
- 2.5.4.2 4-Methylacetophenone [122-00-9], *p*-Tolyl Methyl Ketone 128
- 2.5.4.3 Benzylacetone [2550-26-7], 4-Phenyl-2-butanone 129
- 2.5.4.4 Methyl 2-Naphthyl Ketone, Methyl  $\beta$ -Naphthyl Ketone  
[93-08-3] 129
- 2.5.4.5 Benzophenone [119-61-9], Diphenyl Ketone 129
- 2.5.4.6 5-Acetyl-1,1,2,3,3,6-hexamethylindane [15323-35-0] 130
- 2.5.4.7 4-Acetyl-1,1-dimethyl-6-*tert*-butylindane [13171-00-1] 130
- 2.5.4.8 5-Acetyl-1,1,2,6-tetramethyl-3-isopropylindane [68140-48-7] 131
- 2.5.4.9 1-(5,6,7,8-Tetrahydro-3,5,5,6,8,8-hexamethyl-2-  
naphthalenyl)ethanone [1506-02-1], [21145-77-7],  
6-Acetyl-1,1,2,4,4,7-hexamethyltetraline (AHTN) 132
- 2.5.5 Esters of Aliphatic Alcohols and Aliphatic Acids 133
- 2.5.5.1 Benzyl Acetate [140-11-4] 133
- 2.5.5.2 Benzyl Propionate [122-63-4] 133
- 2.5.5.3 Benzyl Isovalerate [103-38-8] 133
- 2.5.5.4 Phenylethyl Acetate [103-45-7] 134
- 2.5.5.5 Phenylethyl Isobutyrate [103-48-0] 134
- 2.5.5.6 Phenylethyl Isovalerate [140-26-1] 134
- 2.5.5.7 1-Phenylethyl Acetate [50373-55-2], Styrallyl Acetate 134
- 2.5.5.8  $\alpha$ -Trichloromethylbenzyl Acetate [90-17-5] 135
- 2.5.5.9  $\alpha,\alpha$ -Dimethylphenylethyl Acetate [151-05-3] 135
- 2.5.5.10  $\alpha,\alpha$ -Dimethylphenylethyl Butyrate [10094-34-5] 136
- 2.5.5.11 Cinnamyl Acetate [21040-45-9] 136
- 2.5.6 Aromatic Acids 136
- 2.5.6.1 Phenylacetic Acid [103-82-2] 136
- 2.5.7 Esters Derived from Aromatic and Aliphatic Acids 137
- 2.5.7.1 Benzoates 137
- 2.5.7.2 Phenylacetates 138
- 2.5.7.3 Cinnamates 138
- 2.5.8 Miscellaneous Compounds 139

- 2.5.8.1 Musk ketone [81-14-1], 3,5-Dinitro-2,6-dimethyl-4-*tert*-butylacetophenone 139
- 2.5.8.2 Cinnamionitrile [4360-47-8] 140
- 2.5.8.3 3-Methyl-5-phenyl-2-pentenitrile [93893-89-1] 140
- 2.5.8.4 2-Cyclohexylidene-2-phenylacetoneitrile [10461-98-0] 141
- 2.5.8.5 Methyl Anthranilate [134-20-3] 141
- 2.5.8.6 Methyl *N*-Methylantranilate [85-91-6] 142
- 2.5.8.7 2-Ethyl-*N*-methyl-*N*-(3-methylphenyl)butanamide [406488-30-0] 142
- 2.6 Phenols and Phenol Derivatives 143
  - 2.6.1 Phenols, Phenyl Esters, and Phenyl Ethers 143
    - 2.6.1.1 Diphenyl Ether [101-84-8] 143
    - 2.6.1.2 Phenoxyacetic Acid 2-Propenyl Ester [7493-74-5], Phenoxyacetic Acid Allyl Ester 143
    - 2.6.1.3 Thymol [89-83-8], 2-Isopropyl-5-methylphenol 144
    - 2.6.1.4 Anethole [104-46-1], 1-Methoxy-4-(1-propenyl)benzene 144
    - 2.6.1.5 1-(Cyclopropylmethyl)-4-methoxybenzene [16510-27-3] 146
    - 2.6.1.6 2-Phenoxyethyl Isobutyrate [103-60-6] 146
    - 2.6.1.7 Methyl 2-Naphthyl Ether [93-04-9], 2-Methoxynaphthalene, Nerolin Yara-Yara 146
    - 2.6.1.8 Ethyl 2-Naphthyl Ether [93-18-5], 2-Ethoxynaphthalene, Nerolin Bromelia 147
    - 2.6.1.9 Isobutyl 2-Naphthyl Ether [2173-57-1], 2-(2-Methyl-2-propoxy)naphthalene 147
    - 2.6.1.10 Hydroquinone Dimethyl Ether [150-78-7], 1,4-Dimethoxybenzene 147
    - 2.6.1.11 Isoeugenol [97-54-1], 2-Methoxy-4-(1-propenyl)phenol 147
    - 2.6.1.12 Isoeugenol Methyl Ether [93-16-3], Methyl Isoeugenol 148
    - 2.6.1.13 Eugenol [97-53-0], 2-Methoxy-4-allylphenol 148
    - 2.6.1.14 Eugenol Methyl Ether [93-15-2], Methyl Eugenol 149
    - 2.6.1.15 Eugenol Acetate [93-28-7] 149
    - 2.6.1.16 Propenylguethol [94-86-0], 2-Ethoxy-5-(1-propenyl)phenol 150
    - 2.6.1.17 *p*-Cresyl Phenylacetate [101-94-0] 150
  - 2.6.2 Phenol Alcohols and Their Esters 150
    - 2.6.2.1 Anise Alcohol [105-13-5], 4-Methoxybenzyl Alcohol 151
    - 2.6.2.2 Anisyl Acetate [104-21-2] 151
  - 2.6.3 Phenol Aldehydes 151
    - 2.6.3.1 *p*-Anisaldehyde [123-11-5], 4-Methoxybenzaldehyde 151
    - 2.6.3.2 2-Methyl-3-(4-methoxyphenyl)propanal [5462-06-6] 152
    - 2.6.3.3 Vanillin [121-33-5], 4-Hydroxy-3-methoxybenzaldehyde 152
    - 2.6.3.4 Veratraldehyde [120-14-9], 3,4-Dimethoxybenzaldehyde 155
    - 2.6.3.5 Ethylvanillin [121-32-4], 3-Ethoxy-4-hydroxybenzaldehyde 155
    - 2.6.3.6 Heliotropin [120-57-0], Piperonal, 3,4-Methylenedioxybenzaldehyde 156

- 2.6.3.7 2-Methyl-3-(3,4-methylenedioxyphenyl)propanal [1205-17-0] 157
- 2.6.4 Phenol Ketones 157
- 2.6.4.1 4-Methoxyacetophenone [100-06-1], Acetanisole 158
- 2.6.4.2 4-(4-Hydroxyphenyl)-2-butanone [5471-51-2], Raspberry Ketone 158
- 2.6.5 Phenolcarboxylates 158
- 2.6.5.1 Salicylates 158
- 2.6.5.2 Resorcylic Acid Esters 160
- 2.7 O-, O,S- and S,S-Heterocycles 161
- 2.7.1 Cyclic Ethers 161
- 2.7.1.1 1,8-Cineole [470-82-6], 1,8-Epoxy-*p*-menthane, Eucalyptol 162
- 2.7.1.2 Rose Oxide [16409-43-1],  
4-Methyl-2-(2-methyl-1-propenyl)tetrahydropyran 163
- 2.7.1.3 Menthofuran [494-90-6],  
3,6-Dimethyl-4,5,6,7-tetrahydrobenzofuran 164
- 2.7.1.4 Linalool Oxide,  
2-Methyl-2-vinyl-5-( $\alpha$ -hydroxyisopropyl)tetrahydrofuran 165
- 2.7.1.5 6-Butyl-3,6-dihydro-2,4-dimethyl-2H-pyran [24237-00-1] 165
- 2.7.1.6 1,5,9-Trimethyl-13-oxabicyclo[10.1.0]trideca-4,8-diene  
[13786-79-3] 166
- 2.7.1.7 3a,6,6,9a-Tetramethyldodecahydronaphtho[2,1-b]furan [6790-58-5],  
[3738-00-9], Ambergis Oxide 166
- 2.7.1.8 Decahydro-2,6,6,7,8,8-hexamethyl-2H-indeno[4,5-b]furan  
[338735-71-0] 167
- 2.7.1.9 4-Hydroxy-2,5-dimethyl-3(2H)-furanone [3658-77-3], Pineapple  
Ketone 168
- 2.7.1.10 2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone [27538-10-9] and  
5-Ethyl-4-hydroxy-2-methyl-3(2H)-furanone [27538-09-6],  
"Homofuraneol" 169
- 2.7.1.11 Maltol [118-71-8], 3-Hydroxy-2-methyl-4H-pyran-4-one 169
- 2.7.1.12 Ethylmaltol [4940-11-8], 2-Ethyl-3-hydroxy-4H-pyran-4-one 169
- 2.7.1.13 2-Isobutyl-4-methyltetrahydro-2H-pyran-4-ol [63500-71-0] 170
- 2.7.1.14 3-Pentyltetrahydro-2H-pyran-4-ol Acetate [18871-14-2] 170
- 2.7.1.15 4,6,6,7,8,8-Hexamethyl-1,3,4,6,7,8-  
hexahydrocyclopenta[g]benzopyran [1222-05-5],  
"HHCB" 171
- 2.7.1.16 2-Butyl-4,4,6-trimethyl-1,3-dioxane [54546-26-8] 172
- 2.7.1.17 6-Isopropyl-9-methyl-1,4-dioxaspiro[4,5]decane-2-methanol  
[63187-91-7], Menthone Glycerine Acetal 172
- 2.7.1.18 Hexahydro-1',1',5',5'-tetramethyl-spiro[1,3-dioxolane-2,8'(5'H)-  
[2H-2,4a]-methanonaphthalene] [154171-76-3],  
[154171-77-4] 172
- 2.7.1.19 2-(2,4-Dimethyl-3-cyclohexenyl)-5-methyl-5-(1-methylpropyl)-1,3-  
dioxane [117933-89-8] 173

- 2.7.1.20 Dodecahydro-3,8,8,11a-tetramethyl-5*H*-3,5a-epoxynaphth[2,1-*c*]oxepin [57345-19-4], 8,13;13,20-Diepoxy-15,16-dinor-8β*H*-labdane, Ambraketol 173
- 2.7.1.21 (4*aR*,5*R*,7*aS*,9*R*)-Octahydro-2,2,5,8,8,9*a*-hexamethyl-4*H*-4*a*,9-methanozulenol[5,6-*d*]-1,3-dioxole [211299-54-6] 174
- 2.7.1.22 Phenylacetaldehyde glycerine Acetal [29895-73-6], 2-Benzyl-1,3-dioxolan-4-methanol 174
- 2.7.1.23 2,4,6-Trimethyl-4-phenyl-1,3-dioxane [5182-36-5] 175
- 2.7.1.24 4,4*a*,5,9*b*-Tetrahydroindeno[1,2-*d*]-*m*-dioxin [18096-62-3] 175
- 2.7.1.25 4,4*a*,5,9*b*-Tetrahydro-2,4-dimethylindeno[1,2-*d*]-1,3-dioxin [27606-09-3] 175
- 2.7.1.26 7-Methyl-2*H*-1,5-benzodioxepin-3(4*H*)-one [28940-11-6], Watermelon Ketone 176
- 2.7.1.27 Ethyl (2-Methyl-[1,3]dioxolan-2-yl)-acetate [6413-10-1], (2-Methyl-[1,3]dioxolan-2-yl)-acetic Acid Ethyl Ester 176
- 2.7.1.28 Ethyl (2,4-Dimethyl-[1,3]dioxolan-2-yl)-acetate [6290-17-1], (2,4-Dimethyl[1,3]dioxolan-2-yl)-acetic Acid Ethyl Ester 176
- 2.7.1.29 1-(3-Methylbenzofuran-2-yl)-ethanone [23911-56-0] 177
- 2.7.1.30 *cis*-2-Methyl-4-propyl-1,3-oxathiane [59323-76-1] 177
- 2.7.2 Lactones 177
- 2.7.2.1 γ-Octalactone [104-50-7] (R = *n*-CH<sub>3</sub>-(CH<sub>2</sub>)<sub>3</sub>-) 178
- 2.7.2.2 γ-Nonalactone [104-61-0] (R = *n*-CH<sub>3</sub>-(CH<sub>2</sub>)<sub>4</sub>-), the So-Called "Aldehyde C<sub>18</sub>" 178
- 2.7.2.3 γ-Decalactone [706-14-9] (R = *n*-CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-) 178
- 2.7.2.4 γ-Undecalactone [104-67-6] (R = *n*-CH<sub>3</sub>-(CH<sub>2</sub>)<sub>6</sub>-), the So-Called "Aldehyde C<sub>14</sub>" 179
- 2.7.2.5 β-Methyl-γ-octalactone [39212-23-2], Whiskey Lactone 179
- 2.7.2.6 3-Hydroxy-4,5-dimethyl-2(5*H*)-furanone [28664-35-9], Sotolone 179
- 2.7.2.7 5-Ethyl-3-hydroxy-4-methyl-2(5)-furanone [698-10-2], Abhexone, Maple Furanone 180
- 2.7.2.8 δ-Decalactone [705-86-2] 180
- 2.7.2.9 δ-Dodecalactone [713-95-1] 181
- 2.7.2.10 15-Pentadecanolide [106-02-5], 15-Hydroxypentadecanoic Acid Lactone 181
- 2.7.2.11 15-Pentadec-11-enolide/15-Pentadec-12-enolide (Mixture of (*E*)- and (*Z*)-Isomers) [34902-57-3] 183
- 2.7.2.12 9-Hexadecen-16-olide [28645-51-4], Oxacycloheptadec-10-en-2-one, Ambrettolide 183
- 2.7.2.13 Oxa-16-hexadecanolides 184
- 2.7.2.14 1,12-Dodecanedioic Acid Ethylene Ester [54982-83-1] 184
- 2.7.2.15 1,13-Tridecanedioic Acid Ethylene Ester [105-95-3], Ethylene Brassylate (n = 11) 185
- 2.7.2.16 Coumarin [91-64-5], 2*H*-1-benzopyran-2-one 185

2.7.2.17	Dihydrocoumarin [119-84-6], 3,4-Dihydro-2H-benzopyran-2-one	186
2.7.3	Glycidates	187
2.7.3.1	Ethyl 3-Phenylglycidate [121-39-1], the So-Called "Aldehyde C <sub>16</sub> Special"	187
2.7.3.2	Ethyl 3-Methyl-3-phenylglycidate [77-83-8], the So-Called "Aldehyde C <sub>16</sub> ," Strawberry Aldehyde	187
2.7.4	Miscellaneous Compounds	188
2.7.4.1	2-Furylmethanethiol [98-02-2], Furfuryl Mercaptan	188
2.8	N- and N,S-Heterocycles	188
<b>3</b>	<b>Natural Raw Materials in the Flavor and Fragrance Industry</b>	<b>193</b>
3.1	Introduction	193
3.2	Isolation of Natural Fragrance and Flavor Concentrates	194
3.2.1	Essential Oils	195
3.2.2	Extracts	196
3.3	Survey of Natural Raw Materials	197
<b>4</b>	<b>Analytical Methods/Quality Control</b>	<b>265</b>
<b>5</b>	<b>Safety Evaluation and Regulatory Aspects</b>	<b>267</b>
5.1	Flavoring Substances	267
5.2	Fragrance Ingredients	268
	<b>References</b>	<b>271</b>
	<b>Formula Index</b>	<b>317</b>
	<b>Subject Index</b>	<b>341</b>