Identification of Character Impact Odorants of Different White Wine Varieties

H. Guth*

Deutsche Forschungsanstalt für Lebensmittelchemie, Lichtenbergstrasse 4, D-85748 Garching, Germany

Application of gas chromatography/olfactometry (GC/O) to the analysis of extracts of Scheurebe and Gewürztraminer wines yielded 36 and 40 odor-active compounds, respectively. Ethyl 2-methylbutyrate, ethyl isobutyrate, 2-phenylethanol, 3-methylbutanol, 3-hydroxy-4,5-dimethyl-2(5*H*)furanone, 3-ethylphenol, and an unknown compound named wine lactone showed high flavor dilution factors in both varieties. Wine lactone was identified as 3a,4,5,7a-tetrahydro-3,6-dimethylbenzofuran-2(3*H*)-one and was detected for the first time among the volatiles of wine or a food. The compound exhibited an intense coconut, woody, and sweet odor. 4-Mercapto-4-methylpentan-2one belongs to the most potent odorants only in the variety Scheurebe, whereas *cis*-rose oxide was a key substance for the overall flavor of Gewürztraminer wine. GC/O of static headspace samples of both wine varieties revealed butane-2,3-dione, dimethyl sulfide, and dimethyl trisulfide as further potent odorants.

Keywords: Gas chromatography/olfactometry; 3a,4,5,7a-tetrahydro-3,6-dimethylbenzofuran-2(3H)one; cis-rose oxide; 4-mercapto-4-methylpentan-2-one; white wine; flavor; aroma; Gewürztraminer; Scheurebe

INTRODUCTION

To date more than 680 volatile compounds have been identified in different white wine varieties (Maarse and Vissher, 1994). A first approach to distinguish wine varieties on the basis of selected volatiles was carried out by Rapp (1990). According to the pattern of 12 monoterpenes that were detectable in gas chromatograms, he was able to differ between three classes of white wines: Muskat-type, Riesling-type, and Silvanertype.

Systematic studies to indicate the odorants responsible for the characteristic bouquet of wines were performed recently. Using Charm analysis Chrisholm et al. (1994), Schlich and Moio (1994), and Moio et al. (1994) evaluated ethyl hexanoate, ethyl butanoate, and ethyl 2-methylbutanoate as the most potent odorants of Chardonnay and White Riesling wines. Further potent odorants of the variety White Riesling were β -damascenone, 3-methylbutyl acetate, 2-phenylethanol, and linalool. Together with the above-mentioned ethyl esters Moio et al. (1994) evaluated, according to high Charm values, vanillin, butane-2,3-dione, guaiacol, 4-vinylguaiacol, and ethyl cinnamate as further potent odorants of the variety Chardonnay.

Berger (1995) identified (*E*)- β -damascenone and phenylethanol as key odorants of Chardonnay–Semillon wines, as these compounds showed the highest flavor dilution (FD) factors in aroma extract dilution analysis (AEDA).

By application of the Osme technique, Miranda-Lopez et al. (1992) investigated the volatile fractions of different vintages of the variety Pinot Noir. High Osme values were found for 3-methylbutanol, 2-phenylethanol, 2-phenylethyl acetate, hexanoic acid, γ -nonalactone, and 3-(methylthio)-1-propanol.

On the basis of static headspace analysis (SHA), Shimoda et al. (1993) compared wines of one variety from different origins. Leino et al. (1993) used the dynamic headspace technique for the characterization of the flavor of Chardonnay and Semillon wines. In both investigations the authors gave no details about the importance of the recognized compounds, because the gas chromatography analysis was not coupled with sniffing technique.

The aim of the following investigation was to elucidate the most odor-active compounds in Gewürztraminer and Scheurebe wines by the two GC/O techniques AEDA and SHA-O.

EXPERIMENTAL PROCEDURES

Wine. Gewürztraminer, vintage 1992, and Scheurebe wine, vintage 1993, were purchased from a winery in Ballrechten-Dottingen, Germany.

Chemicals. 4-Methyl-3-penten-2-one and sodium hydrogen sulfide were from Aldrich (Steinheim, Germany). Compounds 1–11, 15–22, 25–34, 36, 38, 39, 41, and 43 (Table 1) were also from Aldrich; nerol oxide and compound 12 were from Roth (Karlsruhe, Germany); 13, 23, 37, 42, and 44–46 were from Merck (Darmstadt, Germany); and 24 was a gift from Haarmann and Reimer (Holzminden, Germany).

Synthesis. 4-Mercapto-4-methylpentan-2-one (14). Concentrated H_2SO_4 (2 μ L) was added to acetone (2 mmol, 12 mg), and the mixture was stirred at 25 °C for 24 h. After addition of sodium hydrogen sulfide (1 mmol, 56 mg), the reaction vessel was sealed with a septum and stirred for further 12 h at 25 °C. After addition of water (5 mL), the 4-mercapto-4-methylpentan-2-one (14) formed was extracted with diethyl ether (2 \times 5 mL) and then re-extracted with NaOH (0.1 mol/L, 2 \times 10 mL). Acidification of the aqueous layer with HCl (0.1 mol/L) to pH 3, followed by extraction with pentane (2 \times 10 mL) and drying over Na₂SO₄, yielded 4-mercapto-4-methylpentan-2-one (14, 10 mg).

MS(EI) of 14: m/z (%) 43 (100), 55 (20), 99 (5), 132 (M⁺, 10).

The following odorants were synthesized as reported in the literature: (3.S, 3a.S, 7a.R)-3a, 4, 5, 7a-tetrahydro-3, 6-dimethylbenzofuran-2(3)-one (**37**, wine lactone) (Guth, 1996); dimethyl trisulfide **45** (Milligan et al., 1963); (*Z*)-6-dodeceno- γ -lactone (**40**) (Widder et al., 1991).

Isolation of the Volatile Compounds. *Procedure I.* A solution of wine (100 mL) and NaCl (10 g) was extracted with

^{*} Fax 00498928914183.

Table 1. Intense Odorants of Gewürztraminer and Scheurebe Wines

			RI oi	n	FD-factor ^c		reported as volatile
odorant ^a	$\mathbf{fraction}^b$	FFAP	DB-5	OV-1701	Scheurebe	Gewürztraminer	$\operatorname{compound}^d$
1,1-diethoxyethane (1)	Ν	900	730		1	1	1
ethyl isobutyrate (2)	NI	950	757	812	100	10	1
butane-2,3-dione (3)	NI	967	600	695	1	1	1
ethyl butyrate (4)	NI	1023	804		10	10	1
ethyl 2-methylbutyrate (5)	NI	1055	849	907	100	100	1
ethyl 3-methylbutyrate (6)	NI	1057	853		10	10	1
2-methylpropanol (7)	Ν	1110	647		10	10	1
3-methylbutyl acetate (8)	Ν	1114	880		1	1	1
3-methylbutanol (9)	Ν	1220	736	844	100	100	1
ethyl hexanoate (10)	Ν	1225	1000		10	10	1
octanal (11)	NI	1275	1006	1087	1	1	1
cis-rose oxide $(12)^e$	NII	1337	1112		<1	10	1
hexanol (13)	NIII	1349	870		1	1	1
4-mercanto-4-methylpentan-2-one (14)	NII	1366	944	1063	10	<1	2
(Z)-3-hexenol (15)	NIII	1378	858	1000	1	1	ĩ
ethyl octanoate (16)	N	1423	1200		10	10	1
acetic acid (17)	Δ	1435	1200	805	10	10	3
linalool (18)	NIII	1535	1103	1196	10	10	1
isobutyric acid (10)	Δ	1557	1100	1100	10	1	1
hutvric acid (20)	Δ	1613		1000	10	10	1
2/3 mothylhutyric acid (21)	A A	1657		1040	10	10	1
$2 \pmod{(\mathbf{z})}$		1792	082	1040	10	10	1
sitronallal (92)	NIII	1762	1997			1	1
$(E) \ \rho \ domosconone \ (94)$	NI	1705	1205	1409	~1	1	1
(E) - β -uamascenome (24)	INI N	1000	1393	1490	1	1	4
<i>z</i> -phenyletilyi acetate (<i>z</i> 3)	IN A	1000	1200	1372	1	1	1
nexanoic acid (20)		1030	1959	1184	1 ~1	1	1
geranioi (27)	INIII	1040	1200	1000	<u>_1</u>	1	1
2-methoxyphenol (28)		1840	1090	1229	100	100	1
2-pnenyletnanol (29)		1905	1110	1276	100	100	I r
4-hydroxy-2,5-dimethyl-3(2H)-furanone (HDMF) (30)	AIII	2025	1061	1249	1	1	5
5-ethyl-4-hydroxy-2-methyl-3(2 <i>H</i>)-furanone (EHMF) (31)	AIII	2080	1 4 0 0	1310	10	10	
trans-ethyl cinnamate (32)	NI,11	2125	1460	4500	10	10	1
4-allyl-2-methoxyphenol (eugenol) (33)	NIV	2159	1355	1506	1>	1	1
3-ethylphenol (34)	NIV	2170	1170		100	100	
2-methoxy-4-vinylphenol (vinylguaiacol) (35)	NIV	2192	1315	1480	<1	1	1
3-hydroxy-4,5-dimethyl-2(5 <i>H</i>)-furanone (sotolon) (36)	AIII	2192		1347	100	100	6
wine lactone (37)	NIV	2192	1455		1000	1000	
<i>o</i> -amino acetophenone ^t (38)		2200	1300		1	1	5
decanoic acid (39)	A	2264			1	1	1
(Z)-6-dodeceno- γ -lactone (40)	NV	2396	1657	1894	1	1	
4-hydroxy-3-methoxybenzaldehyde (vanillin) (41)	NV	2596	1412	1633	1	1	1

^{*a*} The compound was identified by comparing it with the reference substance on the basis of the following criteria: retention index (RI) on the capillary columns given in the table, mass spectra obtained by MS(EI) and MS(CI), and odor quality perceived at the sniffing port. ^{*b*} Fraction in which most of the compound appeared after separation in neutral (N) and acidic fraction (A) and additionally after column chromatography on silica gel of the neutral fraction and HPLC on Lichrospher Diol 100 of the acidic fraction, respectively. ^{*c*} Flavor dilution (FD) factor determined in extracts of Gewürztraminer and Scheurebe wines. ^{*d*} Reported in the literature as volatile compound in different white wine varieties. (1) Schreier et al. (1974a–c, 1976, 1977), Schreier and Drawert (1974); (2) Darriet et al. (1993); (3) Van Wyk et al. (1974a,b); (4) Acree et al. (1980, 1993); (6) Masuda et al. (1984). ^{*e*} Separation of the enantiomers was performed on a fused silica capillary coated with the chiral stationary phase octakis(2,3,6-tri-*O*-methyl)- γ -cyclodextrin (Hydrodex γ -PM, 50 m × 0.25 mm; Machery and Nagel, Düren, Germany). Percentages of (-)-(2*S*,4*R*)-rose oxide = 70% of (+)-(2*R*,4*S*)-rose oxide = 30%. ^{*f*} The MS signals were too weak for an unequivocal interpretation. The compound was identified on the basis of the remaining criteria given in footnote *a*.

pentane/diethyl ether (1 + 1, v/v; 2 × 100 mL). The organic layer was washed with brine (2 × 50 mL), dried over Na₂SO₄, and then concentrated to a volume of 1 mL by distilling off the solvent on a Vigreux column (50 × 1 cm) and by micro-distillation (Bemelmans, 1979).

Procedure II. A solution of wine (800 mL) and NaCl (80 g) was extracted with pentane/diethyl ether (1 + 1, v/v; 300 mL) for 6 h using a rotation extraction apparatus (Normag, Hofheim im Taunus, Germany). The extracts obtained in 12 runs were combined, washed with brine (2 × 500 mL), dried over Na₂SO₄, filtered, and concentrated to 100 mL as reported above. The organic phase was treated two times with an aqueous sodium bicarbonate solution (0.5 mol/L; 200 mL), and the organic layer containing the neutral compounds was dried over Na₂SO₄, filtered, and concentrated to 5 mL (fraction N). The bicarbonate solution was adjusted to pH 3.0 with hydrochloric acid (1 mol/L), and the acidic volatiles were then extracted with diethyl ether (200 mL). The extract was dried over Na₂SO₄, filtered, and concentrated to 2 mL (fraction A).

Column Chromatography (CC). Fraction N (1 mL) was applied onto a water-cooled (10–12 °C) column (30 × 1.5 cm i.d.) filled with silica gel 60 [1.5% water, purified according to the method of Esterbauer (1968)]. Elution was performed by using the following solvents: pentane/diethyl ether (200 mL; 95 + 5, v/v; subfraction NI), pentane/diethyl ether (200 mL; 90 + 10, v/v; subfraction NII), pentane/diethyl ether (100 mL; 70 + 30, v/v; subfraction NIV), pentane/diethyl ether (200 mL; 60 + 40, v/v; subfraction NV), and diethyl ether (200 mL; subfraction NVI). The subfractions were concentrated to 100 μ L as described above.

High-Pressure Liquid Chromatography (HPLC). HPLC was performed with the apparatus described previously (Guth and Grosch, 1993a). Fraction A (200 μ L) was separated by HPLC using a Lichrospher 100 Diol column (250 × 4.6 mm, 5 μ m; Bischoff, Leonberg, Germany) with the following solvents: pentane/diethyl ether/methanol (95 + 4.5 + 0.5, v/v/v). The solvent mixture was pumped with a flow rate of 2.0

Table 2. Results of Static Headspace Analysis/Olfactometry (SHA/O) of Scheurebe and Gewürztraminer Wines

	RI		volu	me ^b (mL)
odorant ^a	FFAP	SE-54	Scheurebe	Gewürztraminer
acetaldehyde (42)	<800	<600	2.5 (8) ^c	2.5 (8) ^c
dimethyl sulfide (43)	<800	<600	5.0 (4)	5.0 (4)
ethyl acetate (44)	900	620	20.0 (1)	20.0 (1)
1,1-diethoxyethane (1)	900	730	20.0 (1)	20.0 (1)
ethyl isobutyrate (2)	950	757	0.05 (400)	0.2 (100)
butane-2,3-dione (3)	967	600	10.0 (2)	10.0 (2)
ethyl butyrate (4)	1023	804	0.1 (200)	0.1 (200)
ethyl 2-methylbutyrate (5)	1055	849	0.1 (200)	0.1 (200)
ethyl 3-methylbutyrate (6)	1057	853	10.0 (2)	10.0 (2)
2-methylpropanol (7)	1110	647	20.0 (1)	20.0 (1)
3-methylbutyl acetate (8)	1114	880	0.5 (40)	0.5 (40)
3-methylbutanol (9)	1220	736	0.5 (40)	0.5 (40)
ethyl hexanoate (10)	1225	1000	0.5 (40)	0.5 (40)
octanal d (11)	1275	1006	20.0 (1)	20.0 (1)
<i>cis</i> -rose oxide ^d (12)	1337	1112	>20.0 (<1)	5.0 (4)
dimethyl trisulfide d (45)	1360	970	5.0 (4)	10.0 (2)
4-mercapto-4-methylpentan-2-one ^d (14)	1366	944	10.0 (2)	>20.0 (<1)
ethyl octanoate (16)	1423	1200	0.5 (40)	0.5 (40)
linalool (18)	1535	1103	10.0 (2)	10.0 (2)
(E)- β -damascenone ^d (24)	1795	1395	20.0 (1)	20.0 (1)
2-phenylethanol (29)	1905	1116	5.0 (4)	5.0 (4)
2-methoxy-4-vinylphenol ^d (35)	2192	1315	>20.0 (<1)	5.0 (4)

^{*a*} The compound was identified by comparing its mass spectrum, retention index, and odor quality with the reference compound (cf. Table 1). ^{*b*} Lowest headspace volume required to perceive the odorant at the sniffing port. ^{*c*} Calculated by dividing the largest volume analyzed (20 mL) by the lowest headspace volume required to perceive the odorant at the sniffing port. ^{*d*} MS signals were too weak for an unequivocal interpretation. The compound was identified on the basis of the remaining criteria given in footnote *a*.

mL/min through the column, and the effluent was monitored at 220 nm. Three subfractions with elution ranges of 4-12 mL (AI), 12-24 mL (AII), and 24-44 mL (AIII) were collected from 10 runs.

Enrichment of compound 37 (wine lactone) was achieved by rechromatography of CC subfraction NIV with HPLC using a silica gel column (500 \times 4.6 mm, Shandon Hypersil, 5 μ m; Bischoff, Leonberg, Germany) with pentane/diethyl ether (70 + 30, v/v) as the eluent. The flow rate was 2 mL/min, and the effluent was monitored at 215 nm. The effluent from 20-30 mL was concentrated (100 μ L) and used for further purification by preparative gas chromatography (Guth and Grosch, 1989) on a stainless steel column (3 m \times 2.4 mm) packed with FFAP (10%, w/w) on Chromosorb (WAW DMCS, 80-100 mesh). The following conditions were used: helium as carrier gas (30 mL/min); injector temperature, 200 °C; injection volume, 10 μ L; temperature program, start at 80 °C, hold for 2 min, then raise at 8 °C/min to 250 °C and then keep at 250 °C for 10 min. Compound 37, appearing with a retention time of 15-16 min, was trapped in a water-cooled (5-10 °C) glass spiral. The material obtained from 10 runs was taken up in pentane (200 μ L).

High-Resolution Gas Chromatography (HRGC)/Mass Spectrometry (MS). HRGC was performed with a Type 5300 gas chromatograph (Fisons Instruments, Mainz, Germany) by using the following capillaries: DB-FFAP, DB-1701, and DB-5 (30 m × 0.32 mm, 0.25 μ m film thickness; J&W Scientific, Fisons Instruments, Mainz, Germany). The samples were applied by on-column injection technique at 35 °C and held for 1 min, and then the temperature of the oven was raised at 40 °C/min to 60 °C, held for 1 min, then raised at 6 °C/min to 250 °C, and held for 10 min isothermally.

MS analyses were performed with a MS-8230 (Finnigan, Bremen, Germany) in tandem with the capillaries described above.

The mass spectra in the electron impact mode (MS/EI) were generated at 70 eV and in the chemical ionization mode (MS/ CI) were obtained at 115 eV with isobutane as reagent gas.

Gas Chromatography/Olfactometry (GC/O). The FD factors of potent odorants occurring in the solvent extracts (procedure I) of Gewürztraminer and Scheurebe wines were located by AEDA as recently reported (Ullrich and Grosch, 1987; Guth and Grosch, 1990; Schieberle et al., 1993): The original extract (1 mL) obtained from 100 mL of wine was stepwise diluted with diethyl ether 1:10, 1:100, and 1:1000,

and aliquots (0.5 $\mu L)$ of each fraction were investigated by GC/O on the capillaries detailed in Table 1.

SHA/O were performed as detailed by Guth and Grosch (1993b) for green and black tea samples, with the modification that the glass tube in the desorption heating block of the purge and trap facility was deactivated according the following procedure: The glass tube was put into a sovirel vessel (volume 50 mL), which contained aqueous HCl (9 mol/L, 40 mL); the vessel was sealed with a septum and heated in a drying oven at 120 °C for 12 h. Then the tube was rinsed with aqueous HCl (1 mol/L, 20 mL), dried in a flow of nitrogen gas, and dehydrated in a vacuum drying oven $(3 \times 10^3 \text{ Pa})$ at 230 °C for 1 h. Silanization of the glass tube was performed with a mixture of 1,3-diphenyl-1,1,3,3-tetramethyldisilazane, hexamethyldisilazane, and pentane (1:1:2) for 1 h at 20 °C. Then the tube was dried in a flow of nitrogen gas and heated at 400 °C for 12 h. After cooling at 20 °C, the tube was successively rinsed with toluene (20 mL), methanol (20 mL), and diethyl ether (20 mL).

The wine sample (50 mL) was pipetted into a vessel (volume 200 mL), sealed with a septum, and equilibrated for 10 min at 40 °C. Decreasing headspace volumes (20-0.05 mL) were drawn by a gastight syringe and then analyzed by GC/O (Table 2).

RESULTS AND DISCUSSION

GC/O. The volatile fractions isolated from Gewürztraminer and Scheurebe wines were screened by AEDA for potent odorants. As summarized in Table 2, AEDA yielded 36 and 40 odor active compounds with FD factors in the range of 1-1000 for Scheurebe and Gewürztraminer wines, respectively. Among the perceived odorants there was one compound, 37, showing high FD factors in both varieties. This unknown compound smelled coconut-like, woody, and sweet. After separation of the neutral volatiles from 9.6 L of wine (see Experimental Procedures, procedure II) by column chromatography, HPLC on silica gel, and, additionally, preparative gas chromatography, the mass spectrum, shown in Figure 1, was obtained for compound 37, named wine lactone. This compound, which has not yet been detected in wine or a food flavor, was



Figure 1. Mass spectrum (EI) of wine lactone (37).

identified by application of high-resolution MS and synthesis as 3a,4,5,7a-tetrahydro-3,6-dimethylbenzofuran-2(3*H*)-one. To identify the stereochemistry of wine lactone **37**, which contains three asymmetric carbon atoms, stereochemically controlled syntheses for the eight enantiomers were developed (Guth, 1996). The results of the NMR, MS, CD, and IR measurements, synthesis experiments, and enantioselective gas chromatography demonstrated the identity of compound **37** with the (3*S*,3*a*,*S*,7*a*,*P*)-3*a*,4,5,7*a*-tetrahydro-3,6-dimethylbenzofuran-2(3*H*)-one enantiomer.

Identification experiments of the remaining compounds (Table 1) were started by a separation of the volatiles into the neutral and acidic compounds. Odorants 1, 7–10, 16, 17, 19–21, 25, 26, 37, and 39–41 were detected by HRGC/MS or only by GC/O, as detailed in Table 1, in the neutral (N) and acidic (A) fractions. Compounds 2–6, 11–15, 18, 22–24, 27–36, 40, and 41 were enriched by column chromatography of the neutral fraction and by HPLC of the acidic fraction, respectively, and then analyzed by HRGC/MS.

On the basis of their high FD-factors ethyl 2-methylbutyrate (5), 3-methylbutanol (9), 2-phenylethanol (29), 3-ethylphenol (34), and sotolon (36) were in addition to wine lactone (37) further important odorants in both varieties. With the exception of wine lactone these compounds have also been detected by AEDA as key odorants of Chardonnay-Semillion wine (Berger, 1995). A significant difference between the two varieties was the absence of the black currant-like smelling 4-mercapto-4-methylpentan-2-one (14) in Gewürztraminer wine. 4-Mercapto-4-methylpentan-2-one (14), which showed a high FD factor in the extract of Scheurebe, has also been reported as an important flavor compound of Sauvignon Blanc wine (Darriet et al., 1993). Furthermore, the FD factor of ethyl isobutyrate (2) was higher in the variety Scheurebe (FD = 100) than in Gewürztraminer ($\overrightarrow{FD} = 10$). In contrast to the former, cis-rose oxide (12), citronellol (23), geraniol (27), eugenol (33), and vinylguaiacol (35), exhibiting spicy and flowery odor notes, contributed to the overall flavor of Gewürztraminer wine.

Due to the importance of *cis*-rose oxide (**12**) to the flavor of Gewürztraminer wine, the evaluation of the specific enantiomeric distribution of stereoisomers (–)-(2.S,4.R) and (+)-(2.R,4.S) was of considerable interest. The order of elution of stereoisomers on the chiral stationary phase octakis(2,3,6-tri-*O*-methyl)- γ -cyclodex-trin was assigned according to the guidelines of Werkhoff

et al. (1993). Enantiomeric analysis of Gewürztraminer wine revealed an enantiomeric ratio of (-)-(2S,4R)-*cis*-rose oxide:(+)-(2R,4S)-*cis*-rose oxide of 7:3 (Table 1).

The results of SHA/O analyses are summarized in Table 2. In a 20 mL sample of the air above Scheurebe and Gewürztraminer wines, 20 and 21 odor-active compounds, respectively, were detectable. With the exception of acetaldehyde, ethyl acetate, dimethyl sulfide, and dimethyl trisulfide, the odorants had already been identified by AEDA in the solvent extracts of both varieties (Table 2). On the contrary, compounds **13**, **15**, **17**, **19–23**, **25–28**, **30–34**, and **36–41** were detected only in the solvent extract (Table 1) but not in the headspace samples.

A stepwise reduction of the headspace volume indicated the most potent odorants in the air above the two wines. In 5 mL of injected headspace gas of Gewürztraminer and Scheurebe wines, 12 and 11 odor-active compounds, respectively, were detected. Further reduction to 0.1 mL yielded ethyl butyrate and ethyl 2-methylbutyrate as the most potent odorants in both varieties and, additionally, ethyl isobutyrate in Scheurebe wine.

AEDA and SHA/O yielded the same valuations of compounds **12** and **14**; 4-mercapto-4-methylpentan-2one (**14**) was detected by SHA/O only in the variety Scheurebe and *cis*-rose oxide (**12**) only in the variety Gewürztraminer.

CONCLUSION

This study has revealed potent odorants that are responsible for the overall flavor of Scheurebe and Gewürztraminer wines. AEDA and SHA/O indicated that significant differences in odor profiles of both varieties were mainly caused by *cis*-rose oxide (12) in Gewürztraminer and by 4-mercapto-4-methylpentan-2one (14) in Scheurebe. These compounds are suitable indicators for objectification of flavor differences of the two wine varieties. Wine lactone, which was a further important odorant of both varieties, has not yet been described in the literature among the volatiles of wines or food flavors.

ACKNOWLEDGMENT

I am grateful to Mrs. I. Kirchmann and Mrs. I. Reinhard for skillful technical assistance.

LITERATURE CITED

- Acree, T. E.; Braell, P.; Butts, R. M. The presence of damascenone in cultivars of *Vitis vinifera* (Linneaus), *Rotundifolia* (Michaux), and *Labruscana* (Baily). *J. Agric. Food Chem.* **1981**, *29*, 688–690.
- Bemelmans, J. M. H. In *Progress in Flavour Research*; Land, D. G., Nursten, H. E., Eds.; Applied Science: London, 1979; pp 79–88.
- Berger, R. G. The roots: empirical food biotechnologies and formation of aroma compound. In *Aroma Biotechnology*; Berger, R. G., Ed.; Springer-Verlag: Berlin, 1995; pp 11– 34.
- Chrisholm, M. G.; Guiher, L. A.; Vonah, T. M.; Beaumont, J. L. Comparison of some french-american hybrid wines with White Riesling using gas chromatography-olfactometry. *Am. J. Enol. Vitic.* **1994**, *45*, 201–212.
- J. Enol. Vitic. **1994**, 45, 201–212. Darriet, P.; Tominaga, T.; Demole, E.; Dubourdieu, D. Evidence of the presence of a 4-mercapto-4-methylpentan-2one precursor in Vitis vinifera Sauvignon Blanc grape variety. C. R. Acad. Sci. Paris **1993**, 316, 1332–1335.
- Esterbauer, H. On the autoxidation of methyl linoleate in water. III. Chromatographic separation of water-soluble reaction products. *Fette Seifen Anstrichm.* **1968**, *70*, 1–8.

- Guth, H. Determination of the configuration of wine lactone. *Helv. Chim. Acta* **1996**, *79*, 1559–1571.
- Guth, H.; Grosch, W. 3-Methylnonane-2,4-dione—an intense odour compound formed during flavour reversion of soyabean oil. *Fat Sci. Technol.* **1989**, *91*, 225–230.
- Guth, H.; Grosch, W. Comparison of stored soya-bean and rapeseed oil by aroma extract dilution analysis. *Lebensm. Wiss. Technol.* **1990**, *23*, 59–65.
- Guth, H.; Grosch, W. 12-Methyltridecanal, a species-specific odorant of stewed beef. *Lebensm. Wiss. Technol.* **1993a**, *26*, 171–177.
- Guth, H.; Grosch, W. Identification of potent odorants in static headspace samples of green and black tea powders on the basis of aroma extract dilution analysis (AEDA). *Flavour Fragrance J.* **1993b**, *8*, 173–178.
- Leino, M.; Francis, I. L.; Kallio, H.; Williams, P. J. Gas chromatographic headspace analysis of Chardonnay and Semillion wines after thermal processing. *Z. Lebensm. Unters. Forsch.* **1993**, *196*, 29–33.
- Maarse, H.; Visscher, C. A. *Volatile Compounds in Food, Qualitative and Quantitative Data*, 6th ed.; Central Institute for Nutrition and Food Research, TNO: Zeist, The Netherland, 1994.
- Masuda, M.; Okawa, E.; Nishimura, K.; Yunome, H. Identification of 4,5-dimethyl-3-hydroxy-2(5*H*)-furanone (sotolon) and ethyl 9-hydroxynonanoate in botrytised wine and evaluation of the roles of compounds characteristic of it. *Agric. Biol. Chem.* **1984**, *48*, 2707–2710.
- Milligan, B.; Saville, B.; Swan, J. M. Trisulphides and tetrasulphides from Bunte Salts. J. Chem. Soc. 1963, 3608–3614.
- Miranda-Lopez, R.; Libbey, L. M.; Watson, B. T.; McDaniel, M. R. Odour analysis of Pinot Noir wine from grapes of different maturities by a gas chromatography-olfactometry technique (Osme). J. Food Sci. 1992, 57, 985-1019.
- Moio, L.; Schlich, P.; Etievant, P. Acquisition and analysis of aromagrams of Chardonnay Burgundy wines. *Sci. Aliments.* 1994, 14, 601–608.
- Rapp, A. Natural flavours of wine: correlation between instrumental analysis and sensory perception. *Fresenius' J. Anal. Chem.* **1990**, *337*, 777–785.
- Rapp, A.; Knipser, W.; Engel, L.; Ullemeyer, H.; Heimann, W. Off-flavor compounds in the berry and wine aroma of grape vine hybrids. I. The strawberry-like aroma. *Vitis* **1980**, *19*, 13–23.
- Rapp, A.; Versini, G.; Ullemeyer, H. 2-Aminoacetophenone: the causal agent of the untypical aging flavor (naphthalene note or hybrid note) of wine. *Vitis* **1993**, *32*, 61–62.
- Schieberle, P.; Gassenmeier, K.; Guth, H.; Sen, A.; Grosch, W. Character impact odour compounds of different kinds of butter. *Lebensm. Wiss. Technol.* **1993**, *26*, 347–356.
- Schlich, P.; Moio, L. Correlation between flavour profiles and aromagrams of Chardonnay Burgundy wines. *Sci. Aliments.* 1994, 14, 609–615.
- Schreier, P.; Drawert, F. 3-(Methylthio)-1-propanol, a volatile component of wine-flavour. Z. Lebensm. Unters. Forsch. 1974, 154, 27–28.

- Schreier, P.; Drawert, F.; Junker, A. GLC-mass-spectrometrical investigation of volatile constituents of wine. II. Thiolether-compounds of wines. *Z. Lebensm. Unters. Forsch.* **1974a**, *154*, 279–284.
- Schreier, P.; Drawert, F.; Junker, A. Investigation of volatile components in wine by gaschromatography and massspectrometry. I. Nonpolar compounds of wine-flavour. Z. Lebensm. Unters. Forsch. 1974b, 154, 273–278.
- Schreier, P.; Drawert, F.; Junker, A. GLC-mass-spectrometrical investigation of volatile constituents of wine. V. Alcohols, hydroxy-esters, lactones and other polar compounds of wineflavour. *Chem. Mikrobiol. Technol. Lebensm.* **1974c**, *3*, 154– 160.
- Schreier, P.; Drawert, F.; Junker, A. Identification of volatile constituents from grapes. J. Agric. Food Chem. 1976, 24, 331–336.
- Schreier, P.; Drawert, F.; Junker A. Gaschromatographic determination of volatile components of fermented beverages. X. Quantitative determination of volatile trace components (μg/L) in wines. *Chem. Mikrobiol. Technol. Lebensm.* **1977**, *5*, 45–52.
- Shimoda, M.; Shibamoto, T.; Noble, A. C. Evaluation of headspace volatiles of Cabernet Sauvignon wines sampled by an on-column method. *J. Agric. Food Chem.* **1993**, *41*, 1664–1668.
- Ullrich, F.; Grosch, W. Identification of the most intense volatiles flavour compounds formed during autoxidation of linoleic acid. *Z. Lebensm. Unters. Forsch.* **1987**, *184*, 277–282.
- Van Wyk, C. J.; Kepner, R.; Webb, A. D. Some volatile components of *Vitis vinifera* variety White Riesling. 2. Organic acids extracted from wine. *J. Food Sci.* **1967a**, *32*, 664–668.
- Van Wyk, C. J.; Kepner, R.; Webb, A. D. Some volatile components of *Vitis vinifera* variety White Riesling. 3. Neutral components extracted from wine. *J. Food Sci.* **1967b**, *32*, 669–674.
- Werkhoff, P.; Brennecke, S.; Bretschneider, W.; Güntert, M.; Hopp, R.; Surburg, H. Chirospecific analysis in essential oil, fragrance and flavor research. *Z. Lebensm. Unters. Forsch.* 1993, 196, 307–328
- Widder, S.; Sen, A.; Grosch, W. Changes in the flavour of butter oil during storage—Identification of potent odorants. *Z. Lebensm. Unters. Forsch.* **1991**, *193*, 32–35.

Received for review November 5, 1996. Accepted April 13, 1997. $^{\otimes}$

JF9608433

[®] Abstract published in *Advance ACS Abstracts,* July 15, 1997.