

Odor Characteristics of Aliphatic Metameric C-13 Ketones, Alcohols and Their Derivatives

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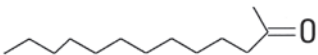
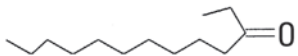
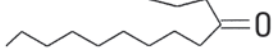
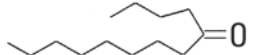
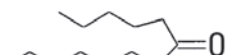
In natural environments, only the tridecanone isomer with the carbonyl group in position 2 has been found to exist. Tridecan-2-one occurs as a flavor component in many raw materials originating from plants or animals, and is produced in multi-step oxidative enzymatic transformations of fatty acids present in them. The presence of tridecan-2-one has been well documented in milk and its products, e.g. in the concentrate of albumen, yogurt, butter and the Italian cheese Grana Padano.^{1,2} Boiled pork liver is also a source of this ketone.³ Tridecan-2-one is present in hop and in a few exotic plants that grow in equatorial or tropic climates. The primary sources of tridecanones and their derivatives are as follows:

- The essential oil from the roots of the plant *Bowdichia virgilioides* (Leguminosae) containing ca. 55 percent tridecan-2-one.⁴
- The essential oil from fresh fruits, flowers and bark of the plant *Litsea monopelata* (Roxb.) containing 11.3 percent tridecanol and 9.4 percent tridecanal.⁵

We recently studied a group of compounds derived from tridecan-7-one and determined their odor characteristics and threshold concentration.⁶ It was discovered that tridecan-7-one and its ethylene acetal have interesting, pleasant nutritive odors. The odors of tridecan-7-ol and its acetate are less interesting — waxy-fatty.

Odor characteristics of tridecan-x-ones (x = 2,3,4,5 and 6)

T-1

Structural formula ^a	Odor characteristics	Odor threshold concentration (ppm)	Reference
	Russian leather with a tanning leather note	20-30	9,10
	Fresh, floral-fatty with an ozone note	10-15	—
	Intensive, warm molten lard	20-30	11
	Intensive, mild with a fatty note	20-30	12
	Fruity with an apple, apricot and musk note	30-40	13

^aFormula: C₁₃H₂₆O; M = 198.35 g·mol⁻¹

The aim of the present work is the determination of the odor of a series of tridecan-x-ones — where x = 2,3,4,5 and 6 — and their derivatives. The relations between structure and odor in the whole family of the tridecanone derivatives are described. The synthesis of all the compounds will be presented in a forthcoming article.⁷



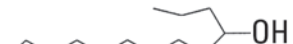
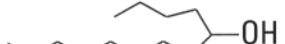

Conclusion

The odor characteristics of ketones and their derivatives are presented in T-1 to T-5. Pleasant notes accompanied fatty-type ketone odors, e.g. floral for tridecan-3-one, and fruity for tridecan-6-one. Alcohols, however, were less interesting, all possessing only a faint or mild waxy odor. Acetates had stronger odors than the corre-

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Odor characteristics of tridecan-x-ols (x = 2,3,4,5 and 6)

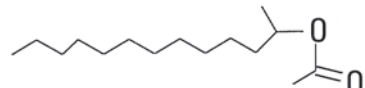
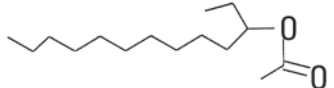
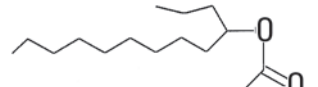
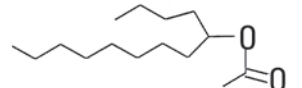
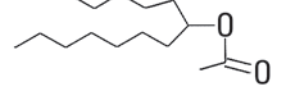
T-2

Structural formula ^a	Odor characteristics	Odor threshold concentration (ppm)	Reference
	Faint waxy, fatty	60-80	—
	Faint, almost odorless	—	—
	Faint waxy, fatty	—	15
	Faint waxy, fatty	60-80	—
	Mild waxy	—	—

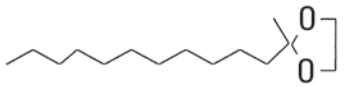
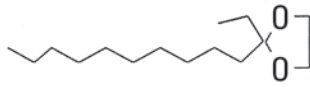
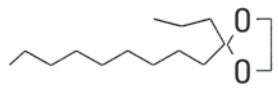
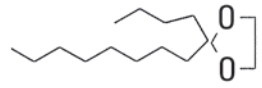
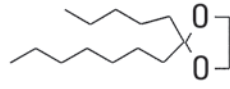
^aFormula: C₁₃H₂₈O; M = 200.36 g·mol⁻¹

Odor characteristics of tridec-x-yl acetates (x = 2,3,4,5 and 6)

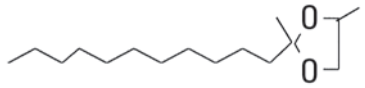
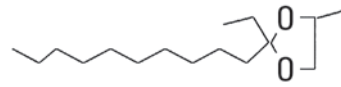
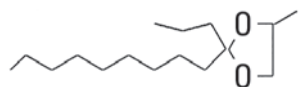
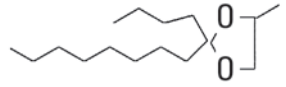
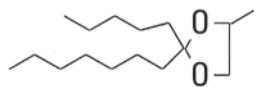
T-3

Structural formula ^a	Odor characteristics	Odor threshold concentration (ppm)	Reference
	Lightly burnt with pineapple note	80-90	15
	Faint, almost odorless	—	—
	Faint, almost odorless	—	—
	Mild, with a blueberry note	40-50	—
	Vegetable with a parsley root note	40-50	—

^aFormula: C₁₅H₃₀O₂; M = 242.40 g·mol⁻¹

Structural formula ^a	Odor characteristics	Odor threshold concentration (ppm)	Reference
	Fresh, light green with a waxy-fatty note	20	—
	Fruity, with a blueberry note	10-15	—
	Faint waxy-fatty	10	—
	Almost odorless	—	—
	Fruity, with a penetrating anise note	10-20	—

^aFormula: C₁₅H₃₀O₂; M = 242.40 g·mol⁻¹

Structural formula ^a	Odor characteristics	Odor threshold concentration (ppm)	Reference
	Faint sweet, fatty-floral	—	—
	Intensive green with sour a note	—	—
	Faint waxy-fatty with an herbaceous note	—	—
	Intensive with a polypore note	20	—
	Fruity-anise with a fatty note	20	—

^aFormula: C₁₆H₃₂O₂; M = 256.43 g·mol⁻¹

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sponding alcohols. Tridec-5-yl and tridec-6-yl acetates had original odors, the former with a pleasant blueberry note, the latter with a vegetable, parsley root note. It is noteworthy that tridecan-3-ol, tridecan-4-ol and their acetates were almost odorless. Acetals were the most interesting group of compounds. They all had nutritive odors with different notes: fruity, spicy, herbaceous or floral, and low odor threshold — 10-20 ppm.⁸

The influence of the position of functional groups in ketones or their derivatives on odor type has been established. The compounds in which the functional group occupies position 2 or 3 have odors with fruity and floral notes. A change in the position of functional groups to 4 or 5 leads to odors with spicy notes. The derivatives of tridecan-6-one have odors with spicy and vegetable notes.

Acknowledgements

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