Aliphatic Monoketones in Flavors

Chemistry and application in flavor

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Ketones are responsible for many natural flavors and odors. Ketones exist in their precursor form in fresh butter as alkanoic acids. As acids, they may be only marginally important in contributing to the flavor of fresh butter. However, when heated, these acid precursors are converted to different ketones and their total concentration rises above their flavor threshold value. Thus, they are very important in providing flavors associated with heated or cooked foods containing butter. Aliphatic ketones are important flavor components, especially in blue cheeses; *Penicillium roqueforti*, for instance, produces 2-pentanone, 2-heptanone and 2-nonanone (**F-1**).[a]

4-Hexen-3-one (FEMA# 3352, CAS# 2497-21-4) (**F-2**), which is this month's aroma ingredient, is a colorless to pale yellow liquid, which has an ethereal, whiskeylike and metallic flavor that is also fruity with tropical nuances,[b] and is applied in vegetable and meaty formulations, as well as rum, butterscotch and horseradish flavors.

4-Hexen-3-one can be prepared from propylene and propionyl chloride by Friedel-Krafts type reaction, firstly to afford 5-chlorohexan-3-one, which loses an HCl molecule by elimination, to give both *trans* and *cis* isomers in *ca.* 9:1 ratio (**F-3**).

The commercial product contains *ca.* 10% of the *cis* isomer.

Another unsaturated ketone for flavors is the homolog 2-octen-4-one (FEMA# 3603, CAS# 4643-27-0) (**F-4**), a clear colorless to pale yellow liquid that occurs in wheaten/soda bread. 2-Octen-4-one has a sweet, fruity, pineapple flavor, and strawberry note with a ripe tropical nuance. It is applied in fruity flavorings, such as strawberry, raspberry, watermelon and tropical fruits.

This molecule can be prepared similarly to 4-hexen-3-one, from propylene and pentanoyl chloride.

Important saturated aliphatic ketones include heptan-2-one, octan-2-one, octan-3-one and nonan-2-one (**F-5**).

Heptan-2-one (methyl amyl ketone; FEMA# 2544, CAS# 110-43-0) occurs in many food flavors, including cereals, dairy, meat and roasted products. It has a spicy, cinnamonlike, cheesy, coconut, waxy flavor and is applied in fruity, cheesy flavors, blue and cheddar cheeses, pineapple, coconut, butter, and banana flavors.

Octan-2-one (methyl hexyl ketone; FEMA# 2802, CAS# 111-13-7) occurs in fries and mushrooms. It has a cheesy, sharp, ketonic flavor with a waxy nuance and is applied in cheese and fruity flavors, blue cheese, cheddar cheese, mushroom, apple, milk and coconut flavors.

The isomer, octan-3-one (ethyl pentyl ketone; FEMA# 2803, CAS# 106-68-3) has a somewhat different flavor, described as fatty, green, fruity, waxy, ketonic, mushroom with a musty cheese nuance.

Nonan-2-one (methyl heptyl ketone; FEMA# 2785, CAS# 821-55-6) has a creamy, fatty, cheesy, fruity, floral organoleptic character. It occurs in many food flavors: fruits, baked, dairy and alcoholic products, meat, and so on. It has a green fruity, dairy, cheesy, buttery flavor; nonan-2-one is applied in fruit and dairy, coconut, cheese, fat and pineapple flavors.

Other ketones are also used as flavor ingredients. Some of these aliphatic ketones are natural flavoring materials,

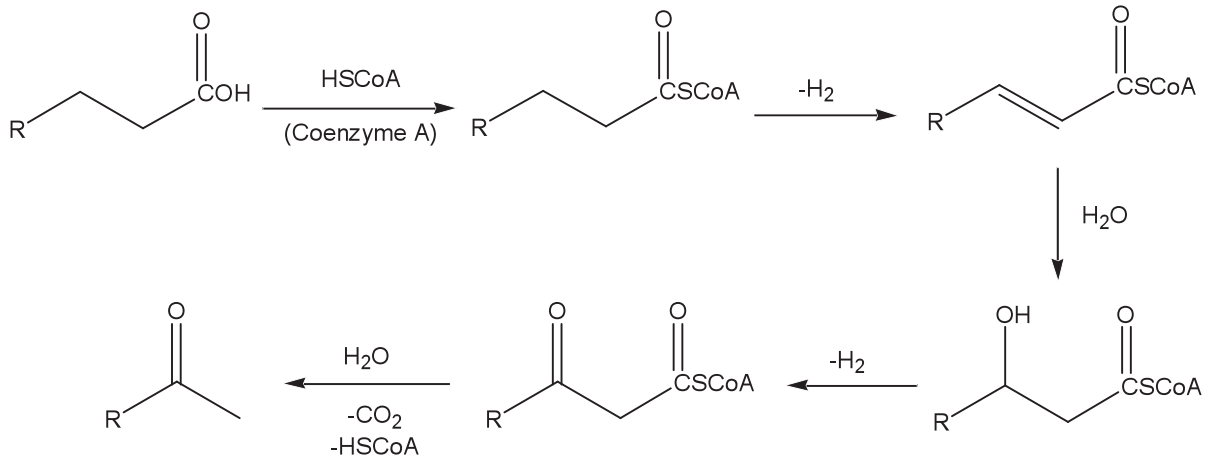
Physical Data for 4-hexen-3-one

Appearance: Colorless to pale yellow liquid
Molecular weight: 98.14
Molecular formula: $C_6H_{10}O$
Refractive index (NaD 20°C): 1.435–1.441
Specific gravity at 20°C: 0.802–0.822
Flashpoint (closed cup): 32°C

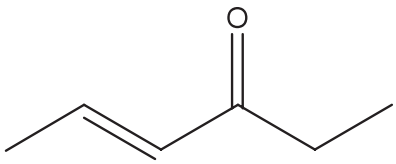
[a] WebExhibits, a public service of the Institute for Dynamic Educational Advancement (IDEA).

[b] Most of the information on organoleptic properties and uses are taken from FRM 2001 and PMP 96 *Databases of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands, and from producers' specification sheets.

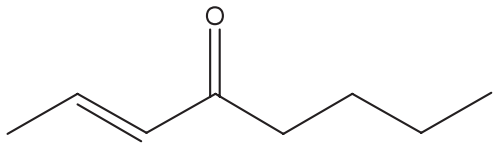
Biochemical pathway for *Penicillium roqueforti* F-1



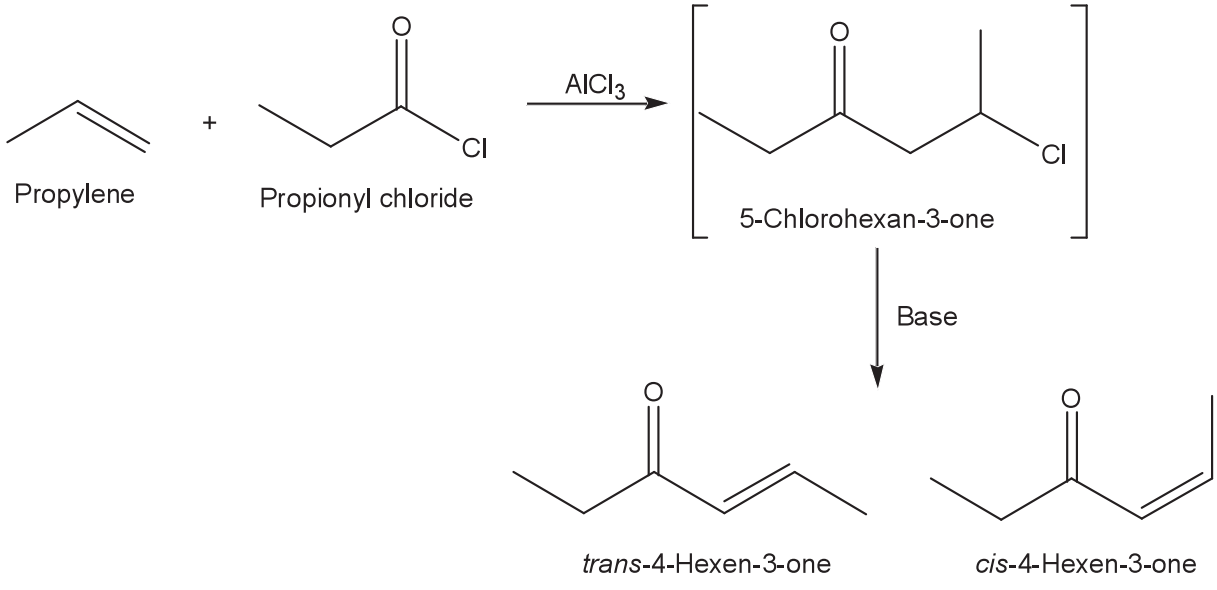
4-Hexen-3-one, *trans*-4-hexene-3-one F-2



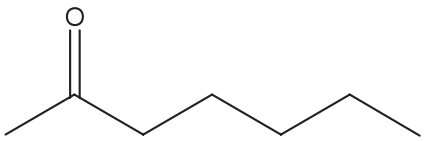
2-Octen-4-one F-4



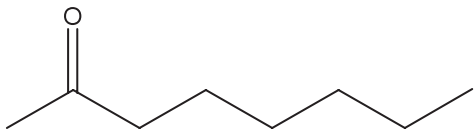
4-Hexen-3-one preparation from propylene and propionyl chloride by Friedel-Krafts reaction F-3



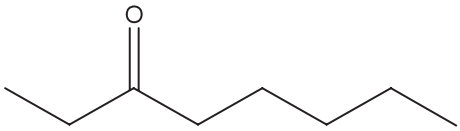
Important saturated aliphatic ketones **F-5**



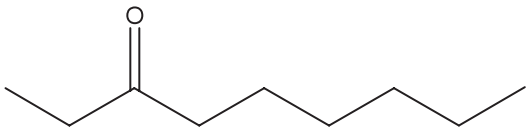
Heptan-2-one



Octan-2-one



Octan-3-one



Nonan-2-one

produced by bio-fermentation and isolated by fractional distillation.

Natural methyl ketones are also produced as a mixture; such a product has a creamy, fruity, tropical, cheesy flavor.

And no review would be complete without mentioning 2-hydroxy-3-butanone (acetoin) and the α-diketones family, *e.g.* diacetyl. These series were shortly reviewed in a former publication.[1]

Reference

1. M. Zviely, 2,3-Pentanedione (Acetyl propionyl), *Perfumer & Flavorist*, July 2009.