2-Methyltetrahydrofuran-3-one and Other Flavor Furans

Chemistry and application in flavors

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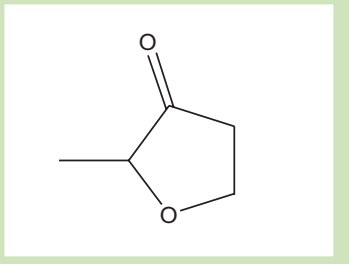
2-Methyltetrahydrofuran-3-one (**F-1**) occurs in coffee, roasted filberts, beer, rum, roasted almonds, potato chips, tobacco, soy sauce and dried scallops.[1–4] It has a breadlike odor, buttery top note, and is nutty and astringent with a slight creamy almond nuance[a]. 2-Methyltetrahydrofuran-3-one is applied in roasted flavorings; almond, rum, cocoa, brandy and caramel flavors; and also in bakery, beef, chocolate, coffee and dairy products.

2-Methyltetrahydrofuran-3-one **F-1**



2-Methyltetrahydrofuran-3-one is called coffee furanone because of its formation during coffee (*Coffea arabica* L.) roasting, as shown by Ruiz et al.[5] Those authors' work showed that furfural (CAS# 98-01-1; **T-1**), 2-methyltetrahydrofuran-3-one and 2,3-pentanedione (CAS# 600-14-6) comprised the majority of the roasted coffee volatiles when heated at 230°C for 8 min. When the roasting lasted an additional 2 min, more molecules were produced, including 2-furanmethanol (CAS# 98-00-0; **T-1**), 2-methyl pyrazine (CAS# 109-08-0), 2,6-dimethyl pyrazine (CAS# 108-50-9) and 2-furanmethanol acetate (CAS# 623-17-6; **T-1**).

2-Methyltetrahydrofuran-3-one is also formed during the Maillard reaction of cysteine and thiamine with reducing sugars. Maillard reactions are known to be important for the aroma generation both in meat and meatlike process flavorings, and are illustrated in **F-2**.

In his work on Maillard reactions and the roles of xylose and thiamine as key starting materials for flavor formation, Cerny used headspace SPME analysis in combination with GC/MS to analyze the volatiles produced from a solution of 13C5-xylose (CAS# 58-86-6)[b], cysteine (CAS# 52-90-4)[c] and thiamine (CAS#59-43-8).[6] These ingredients were heated at 145°C for 20 min and tested by headspace SPME analysis in combination with GC/MS to evaluate the volatiles formed. The resulting furfural and 2-furfuryl mercaptan (CAS# 98-02-2) were 13C5-labeled and hence stemmed from xylose, whereas other formed volatiles, i.e. 2-methyltetrahydrofuran-3-one, 3-mercapto-2-butanone (CAS# 40789-98-8), 4,5-dihydro-2-methyl-3-furanthiol (2-methyl-4,5-dihydrofuran-3-thiol; CAS# 26486-13-5) and 4,5-dihydro-2-methyl-3(2H)-thiophenone (2-methyl tetrahydro-thiophen-3-one; CAS# 13679-85-1) were virtually unlabeled, suggesting their origin from thiamine (**T-2**). Xylose and thiamine were equally important for the formation of 2-methyl-3-furanthiol (CAS# 28588-74-1) and 3-mercapto-2-pentanone (CAS# 67633-97-0) when cysteine was present in the reaction (**F-3**).

Another type of Maillard-browning dairy-type system was studied by Ferretti and Flanagan.[7] This dairy-type system consisting of lactose (CAS# 63-42-3) and casein (CAS# 9000-71-9) produced several compounds that were isolated and identified from a cold finger molecular distillate obtained from a dichloromethane extract of the product. The experiment was done in connection with studies on off-flavor development in dairy products. 2-Methyltetrahydrofuran-3-one was one of several other flavor molecules formed in this dairy system, in a relatively

Physical Data for 2-Methyltetrahydrofuran-3-one

- Synonyms: Coffee furanone, sugar furanone
- $C_5H_8O_2$
- CAS# 3188-00-9
- FEMA# 3373
- Appearance: Colorless to pale yellow liquid
- M.W.: 100.1
- Specific gravity: 1.0340°–1.0450 25°C
- Refractive index: 1.4290°–1.4304 20°C
- Boiling point: 138°–139°C
- Flash point: 40°C TCC (103°F)
- logP (o/w): -0.65 (estd.)

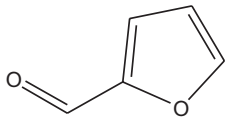
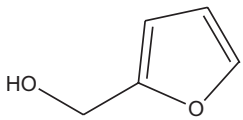
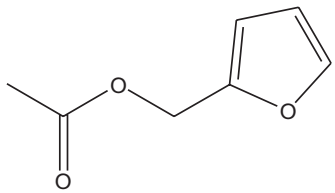
[a] Some of the information on organoleptic properties and uses are taken from sources such as FRM 2001 and PMP 96 Databases of Perfumery Materials & Performance, Boelens Aroma Chemicals Information Services, The Netherlands

[b] CAS# of D-xylose

[c] CAS# of L-cysteine

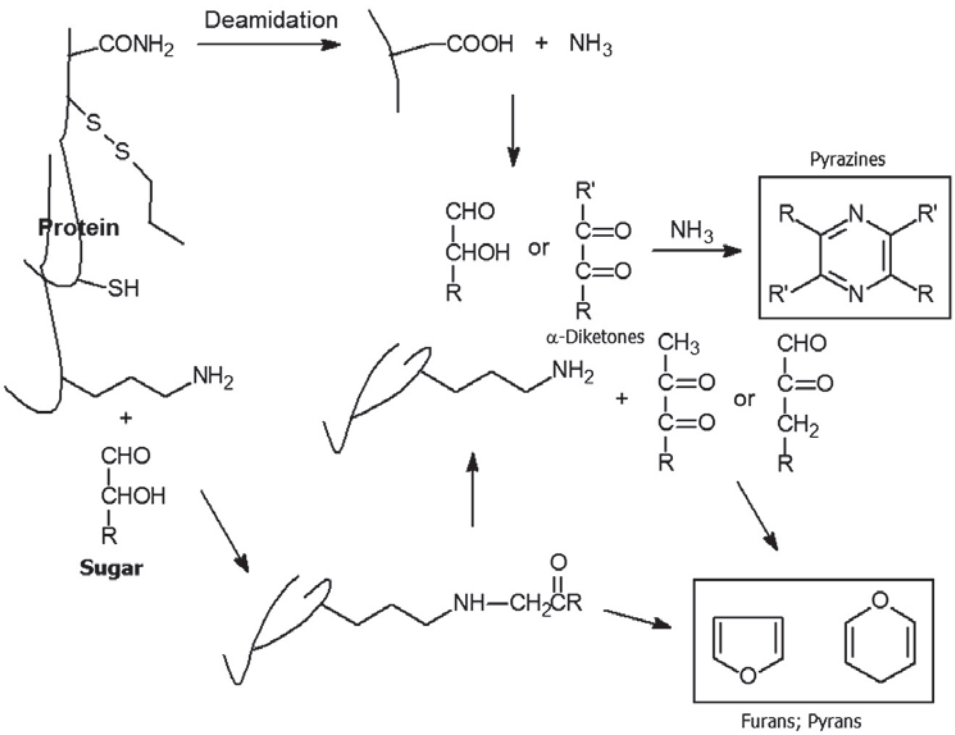
Furfural, 2-furanmethanol and 2-furanmethanol acetate

T-1

Furan Ingredients	Structure	Organoleptic Properties
Furfural		Sweet caramellike, nutty, baked bread, almond
2-Furanmethanol (furfuryl alcohol)		Burnt, sweet, caramellic, brown
2-Furanmethanol acetate (furfuryl acetate)		Fruity, bananalike

The Maillard reaction of cysteine and thiamine with reducing sugars

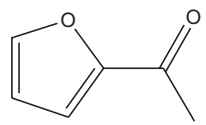
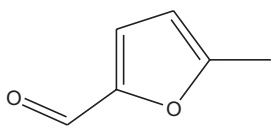
F-2



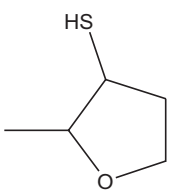
Furan ingredients and their organoleptic properties **T-2**

Furan Ingredient	Organoleptic Properties
2-Furfuryl mercaptan	On dilution strong coffeelike; sulfurous, roasted, onion, garlic
4,5-Dihydro-2-methyl-3-furanthiol	Sulfurous, burnt and roasted on dilution
2-Methyl tetrahydro-thiophen-3-one	Slightly sulfurous and fruity; fried meat on dilution
2-Methyl-3-furanthiol	Sulfurous, coffee- and meatlike on extreme dilution; fishy, salmon and tunalike with a slightly roasted nuance

Possible synthetic pathways toward 2-methyltetrahydrofuran-3-one **T-3**

Furan Ingredients	Structure	Organoleptic Properties
2-Acetylfuran		Sweet aromatic, ethereal, musty, caramel, somewhat bitter almondlike
5-Methyl-2-furaldehyde (5-methylfurfural)		Sweet, caramellic, brown, grain, maplelike

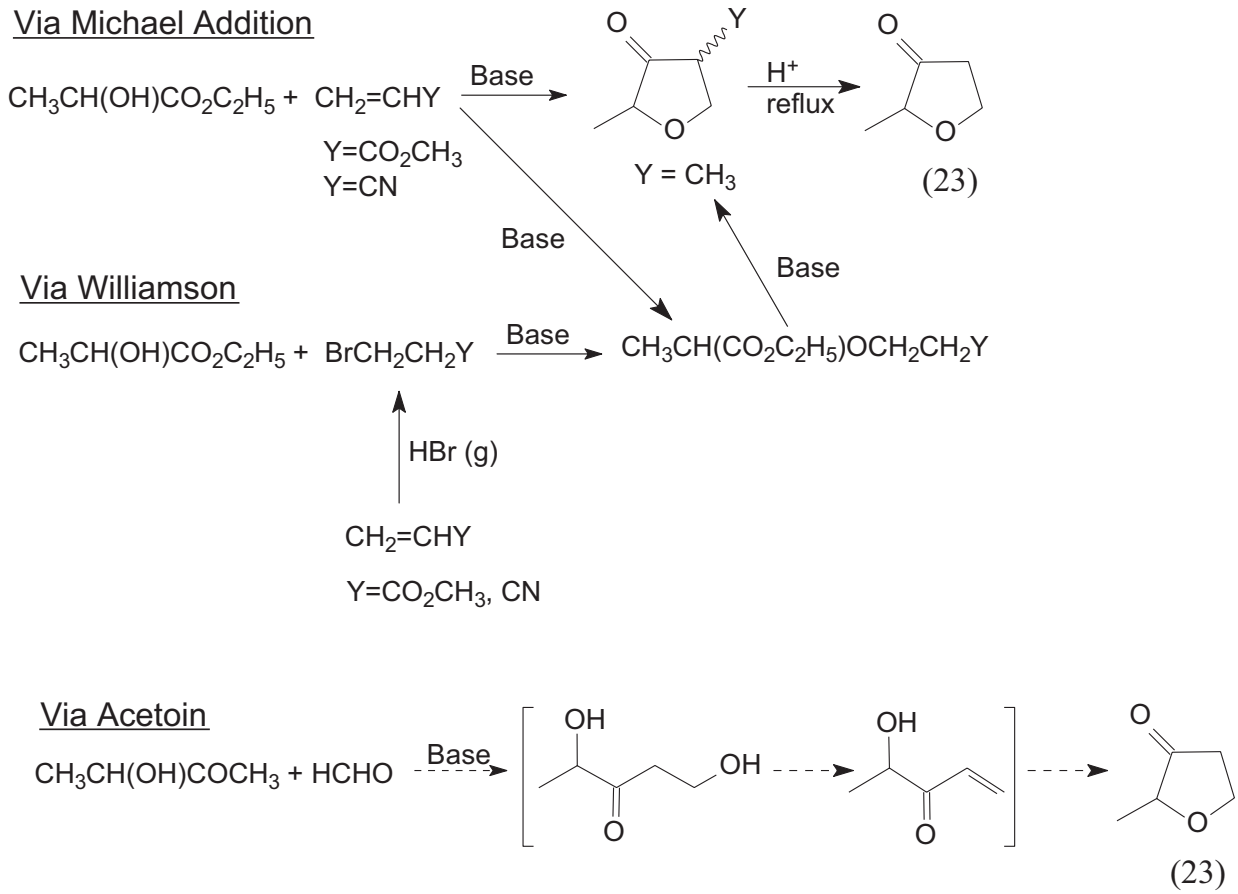
2-Methyl-3-tetrahydrofuran thiol **F-3**



high concentration, as can be observed from the GC of the extract; however, 2-acetyl furan (CAS# 1192-62-7), 5-methyl-2-furaldehyde (CAS# 620-02-0), furfuryl acetate and furfuryl alcohol were present in the largest concentrations (**T-3**).

Another important furan derivative is 2-methyl-3-tetrahydrofuran thiol (CAS#57124-87-5; **F-3**). Even 0.10% in ethanol solution imparts a strong roasted meat, cooked onion and garlic flavor to products when used at levels of 10–100 ppb. 2-Methyl-3-tetrahydrofuran thiol is not yet reported as being found in nature, but it is probably formed in cooked meat. This ingredient has a roast beef, meaty flavor, with brothy savory chicken and turkey notes; it has a slight fatty alliaceous onion and garlic nuances, and it is mostly used in meat formulations.[8]

Possible synthetic pathways toward 2-methyltetrahydrofuran-3-one **F-4**



Some possible synthetic pathways toward 2-methyltetrahydrofuran-3-one are shown in **F-4**.[9]

References

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