Flavor Bites: 2-Methyl-4-propyl-1,3-oxathiane

Use in tropical, citrus, berry and other fruit flavors

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Catty notes have a proud history of use in flavors, especially in fruit flavors. Buchu oil (FEMA# 2169, CAS# 68650-46-4) was for many years the dominant note in blackcurrant flavors and an important note in many others. Unfortunately, buchu oil had some practical disadvantages. It contained a significant level of isomenthone (FEMA# 3460, CAS# 491-07-6) and menthone (FEMA# 2667, CAS# 89-80-5). This gave it a noticeable peppermint note that was often unwelcome in fruit flavor profiles. This problem was soon resolved by using the single ingredient responsible for the catty note, p-mentha-8-thiol-3-one (FEMA# 3177, CAS# 38462-22-5). This leads us to the second problem. p-Mentha-8-thiol-3-one, either from buchu oil or synthesized, decomposed quite readily, and the catty note tended to fade on storage. The third disadvantage was the fact that many flavor types where it was used required a hint of metallic character in addition to the catty note in order to be judged authentic. This was especially true of grapefruit and passion fruit flavors. The problem could be solved by adding small quantities of alternative catty notes that were much more metallic in nature, such as 1-hexanethiol (FEMA# 3842, CAS# 111-31-9) and 1-heptanethiol (FEMA# 4259, CAS# 1639-09-4). Unfortunately, these sulfur compounds were more stable than p-mentha-8-thiol-3-one, and the end result became unpleasantly metallic on storage.

Several terpene sulfur chemicals were developed that possessed a more or less ideal balance between catty and metallic notes, such as 2-pinane thiol (FEMA# 3503, CAS# 23832-18-0) and p-menthene-8-thiol (FEMA# 3700, CAS# 71159-90-5). These chemicals were effective, especially in grapefruit flavors, but still tended to break down, losing H_2S, in much the same way as p-mentha-8-thiol-3-one. In my opinion, 2-methyl-4-propyl-1,3-oxathiane (FEMA# 3578, CAS# 59323-76-1) offers the best solution to this dilemma. It has an ideal balance of catty and metallic notes for passion fruit and grapefruit flavors, and it is far more stable in use than any of the alternatives. The metallic character of this chemical is little more than a hint in relation to the strong catty note, but where it needs to be reduced further, a 40:60 blend with p-mentha-8-thiol-3-one offers a good compromise between character and stability. A few other oxathiane catty sulfur chemicals have been developed over the years, most notably 2-ethyl-4,4-dimethyl-1,3-oxathiane and 4-methyl-2-propyl-1,3-oxathiane (FEMA# 4677), but 2-methyl-4-propyl-1,3-oxathiane remains the most effective member of this family of chemicals.

Tropical Flavors

Pineapple: 2-Methyl-4-propyl-1,3-oxathiane is one of the most important components of pineapple in nature. In this flavor category, it is almost always used in conjunction with methyl 3-methyl thiopropionate (FEMA# 2720, CAS# 13532-18-8) and ethyl 3-methylthiopropionate (FEMA# 3343, CAS# 13327-56-5). The level of use of all three sulfur chemicals varies considerably depending on the level of freshness or canned character required in the flavor. Ten ppm is a good starting point in a flavor intended for use at 0.05% in a ready-to-drink beverage, but levels up to 200 ppm can be accommodated in flavors with a more juicy character. Higher overall levels of all three sulfur chemicals tend to give the flavor a

more processed note. A higher ratio of 2-methyl-4-propyl-1,3-oxathiane to the two thiopropionates tends to push the profile in the opposite direction and increase freshness.

Passion fruit: 2-Methyl-4-propyl-1,3-oxathiane is an even more important natural component of passion fruit. The slightly metallic, catty note is perfect for this flavor. One hundred ppm in a flavor is a good starting point. Combinations with 3-mercaptohexanol (FEMA# 3850) are particularly interesting in passion fruit flavors. This chemical also has catty and metallic notes and adds authenticity in this specific flavor category. It suffers from a degree of instability and should be used with care in challenging applications.

Lychee: Lychee flavors can easily be overcome by their dominant rose character; a subtle addition of this ingredient, around 1 ppm in a flavor, adds complexity and considerable realism.

Mango: The sulfur notes used in mango can be quite complex, mainly catty, and almost form a little flavor all by themselves. The metallic note is not only subtle, but blends well with the oxide notes of mango skin. Three ppm in a flavor is a good initial level.

Guava: Slightly more robust levels are desirable in realistic guava flavors. Ten ppm makes a good starting point in a flavor, but much higher levels are possible in very ripe flavors.

Citrus Flavors

Grapefruit: This chemical is not, to my knowledge, found in grapefruit juice, but it is almost perfectly suited to grapefruit flavors. Higher levels give a more juicy character and a good starting range is 5–30 ppm in a flavor. Grapefruit flavors are especially vulnerable to stability concerns, and 2-methyl-4-propyl-1,3-oxathiane ensures that some recognizable character remains even in difficult beverage storage conditions.

Mandarin: After grapefruit, these flavors are the most interesting citrus application of this raw material. Twenty ppm is a good place to start, but higher levels are possible in juicy mandarin flavors.

Tangerine: Tangerine flavors typically require lower levels of this ingredient than mandarin flavors, usually between 5 and 10 ppm.

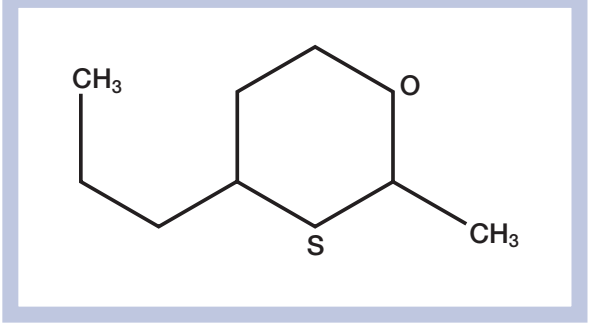
Orange: More subtle levels are useful in orange flavors, typically up to around 5 ppm, adding freshness and impact. Higher levels should be avoided, as they can easily steer the flavor in the direction of grapefruit.

Lemon: Levels of use are very similar in lemon flavors, from 1–5 ppm. They add freshness and lemon juice character and can be exceptionally helpful because they help integrate high (but attractive) levels of addition of methyl jasmonate (FEMA# 3410) or methyl dihydrojasmonate (FEMA# 3408, CAS# 24851-98-7).

Berry Flavors

Blackcurrant: 2-Methyl-4-propyl-1,3-oxathiane can be used alone very successfully in fresh blackcurrant flavors at levels of 10–100 ppm, depending on the degree of sulfur character required. Blends with p-mentha-8-thiol-3-one are also highly attractive, especially where a more processed note is needed.

Structure of 2-Methyl-4-propyl-1,3-oxathiane **F-1**



4-Methoxy-2-methyl butane-2-thiol (FEMA# 3785, CAS# 94087-83-9) and several related chemicals have attractive catty notes that work well in fresh blackcurrant flavors, but they are relatively unstable and also benefit from being used in conjunction with 2-methyl-4-propyl-1,3-oxathiane.

Strawberry: Levels around 10 ppm can add noticeable impact and freshness to strawberry flavors, and higher levels can be used in wild strawberry flavors.

Raspberry: A good starting point in fresh raspberry flavors is 4 ppm. At this level, the chemical adds realism and fresh impact without being overtly sulfuric.

Blackberry: Even lower levels are ideal in fresh blackberry flavors, around 2 ppm. Higher levels should be avoided.

Other Flavors

Peach: Ripe white and yellow peach flavors need a noticeable catty note, and 2-methyl-4-propyl-1,3-oxathiane has the ideal character to convey both ripeness and juicy freshness. Ten ppm in a flavor is a good initial level.

Apricot: Apricot flavors do not so easily accommodate catty notes, and 1 ppm is a good place to start.

Nectarine: Similarly, nectarine flavors benefit from a subtle addition of this ingredient, around 2 ppm.

Rhubarb: The character of 2-methyl-4-propyl-1,3-oxathiane blends particularly well with the dominant notes in rhubarb flavors and up to 10 ppm can be used.

Muscat grape: The best level of use in white grape flavors is 1 ppm, rising to 3 ppm in flavors with an obvious Muscat character.

White wine: Subtle levels, around 1 ppm, can be very helpful in creating white wine flavors. Slightly higher levels are possible where a specifically sauvignon blanc character is the target. The slight catty note offsets the dominant lavender character.

Black tea: Black tea also naturally has a dominant lavender character, and additions in the region of 1 ppm can add impact and realism.

Earl Grey tea: Much higher levels, around 10 ppm, are a useful adjunct to the high levels of bergamot oil used in Earl Grey tea flavors. This ingredient blends especially harmoniously when the flavor also contains small additions of clary sage oil.