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Marketing of an Aliphatic Nitrile for use as a Lemon Bleach Fragrance

Once a chemical company has developed a new compound or formulation, a business case must be prepared to support its full-scale manufacture and commercialisation. As part of a business case, a marketing strategy must be prepared. In this exercise, you are asked to consider the issues relevant to a marketing strategy for the commercialisation of an aliphatic nitrile, either 3-methyloctanonitile, 3-methyldecanonitrile or 2-methyldecanonitile, suitable for use as a fragrance component in lemon bleach (see Lemon Bleach Scenario). Some background information on these nitriles is described in the US patent number 4,579,680 by Charles Sell (*below*). Using your general knowledge of the marketing of chemicals and household products and the marketing models described in this section, the 4Ps model, Product Life Cycle, SWOT model and Porters 5 forces model to guide your thoughts, decide how you will market the aliphatic nitriles and/or the cleaning products incorporating them*. A few thoughts on how to apply the marketing models are provided below.

The 4Ps Model:
This model provides four categories of ***product***, ***price***, ***place*** and ***promotion*** to consider for the aliphatic nitriles. The best way of thinking about each section is to add the word "policy" to each of the words. So for example price "policy" will mean how you are going to price the product in the marketplace. You may have evaluated your costs (see Money section) and wish to add on a profit margin but how much, 5%, 10%, 50%, 100%? However, whatever your costs of manufacture, the price you will be able to obtain in the marketplace will depend on many factors including the market structure (see Market models in Money section) and the economic power within the supply chain (see Porters model). So, are you going to set a high price or a low price relative to other competitive fragrance products? Also for example promotion "policy" will mean where and how you will advertise and promote your product. Will you sell a chemical ingredient to a bleach manufacturer, or a more complex fragrance formulation, or a finished beach direct to retailers?
How will you advertise, by personal selling to large corporate buyers or in chemical catalogues or via national televisions adverts?

Product Life Cycle:
The position of your product within a product life cycle will help you to decide how to market your aliphatic nitrile and where any investment in production, process improvement or logistics may be needed.

SWOT Model:
This model should really be applied to a specific real-life organisation and marketplace so that the ***strengths***, ***weaknesses***, ***opportunities*** and ***threats*** are real. However, in this case study you are asked to propose what aspects of each of the four categories

would be “good and profitable” for the company commercialising aliphatic nitriles and what would be “bad for profitability”. Identify what factors would be good or bad using the information you know about the aliphatic nitriles and any general marketing information you can find on the internet about the fragrance and household bleach markets. This will show what issues will need to be addressed within a marketing strategy.

Porters 5-Forces Model:
Like the SWOT model, for each of the four categories of this model, ***power of suppliers*** and ***buyers***, ***threat of new entrants*** and ***substitutes*** and ***industry structure***, you should propose what aspects would be “good and profitable” for the company commercialising aliphatic nitriles and what would be “bad for profitability”.

Output: Prepare a 2 or 3 page marketing strategy document for the commercialisation of aliphatic nitriles for use as a lemon bleach fragrance. This should include an introduction, a description of output from each marketing model and a concluding statement of critical success factors for the commercialisation of the aliphatic nitriles. Critical success factors are perhaps 5 or 6 key issues that would need to be addressed or put in place before the product should be launched to give it a reasonable chance of commercial success. A new product is more likely to be successful if the company has ***competitive advantage*** over the other suppliers of the product or similar products. Competitive advantage means that a company can offer a product or supporting benefits that competitors are unable to deliver or would find it very expensive to do so, hence commercially unattractive for them to compete with your product. How would you ensure that your aliphatic nitrile has competitive advantage within the bleach market?

* The ‘Lemon Bleach Scenario’ suggests that you produce the nitrile fragrance component in-house and buy in other fragrance components and unfragranced cleaning products in order to formulate your own range of cleaning products for retail. For this Marketing exercise, you can assume this to be true, in which case the exercise is directed at the marketing of your retail product range, ***or*** you can imagine that you are selling the novel nitrile fragrance component to existing cleaning product manufacturers to fragrance their products. This would be a different marketing exercise that might not involve direct marketing to the public. Perhaps you could consider ***both*** situations and this might help you think which would be the best strategy for your new business – concentrating on making the novel fragrance component and selling it to end-users, or making the component and exploiting its novelty in your own range of cleaning products.

United States Patent [19]

Sell

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[54] **ALIPHATIC NITRILES**

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[58] **Field of Search** ..... 252/522 R; 260/465.1

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[57] **ABSTRACT**

This invention provides perfume compositions containing certain substituted saturated aliphatic nitriles and some novel nitriles useful as perfumery components.

1 Claim, No Drawings

ALIPHATIC NITRILES

This is a continuation of application Ser. No. 413,446, filed Aug. 31, 1982, now abandoned.

This invention relates to substituted saturated aliphatic nitriles, more particularly to alpha- and beta-substituted nitriles which have been found to have value in perfume compositions.

Various substituted aliphatic nitriles have been known for some years, but hitherto their value as perfume components has not been appreciated. Our work has shown that certain of the alpha- and beta-substituted aliphatic nitriles, some of which are novel, have particular merit in perfumery compositions.

Accordingly, the present invention provides a perfume composition comprising perfume components and an organoleptically discernible amount of a nitrile of the formula:

$$CH_3(CH_2)_nRCN$$

in which

R=—$CHCH_3$— or —$CHCH_3CH_2$— and in which, when

R=—$CHCH_3$—, n is an integer from 5-9 and when

R=—$CHCH_3CH_2$—, n is an integer from 4-8.

In addition, this invention provides certain novel substituted nitriles of particular value in perfume formulations, having the formula:

$$CH_3(CH_2)_nCHCH_3CH_2CN$$

in which n is 6, 7 or 8.

The nitriles useful in perfume compositions provided by this invention have, in addition to their useful odour characteristics, good stability when used in perfume formulations which are to be used or stored in an aggressive environment, such as in soaps, disinfectants, laundry powders and other compositions in which active chemicals are present or which have to withstand the effects of daylight or heat.

The nitriles useful according to this invention may be prepared by various processes, but a convenient process for the preparation of the alpha-substituted nitriles is as follows:

Procedure A

A solution of the required methyl alkyl ketone (50 m mol) and tosylmethylisocyanide (12 g, 60 m mol) in dry diglyme (120 ml) was added over 15 minutes at 0° C. under nitrogen to a stirred solution of potassium t-butoxide (freshly prepared from potassium 4.3 g, 0.11 g atom) in dry t-butanol (100 ml) and diglyme (100 ml). When the addition was complete, the mixture was allowed to warm to room temperature then stirred for 2 hours and left to stand overnight. The resultant solution was poured into water (400 ml) and extracted with light petroleum (3×100 ml, bp 40°-60° C.). The combined organic extracts were washed with water (2×500 ml), then brine (500 ml) and dried ($MgSO_4$). The solvent was removed under reduced pressure and the residue chromatographed using a column (3 cm diameter, 30 cm height) of silica gel with 5% ether in light petroleum (bp 40°-60° C.) as solvent. Those fractions containing the product were freed of solvent under reduced pressure and the residue distilled to give the desired 2-methyl substituted nitrile.

A convenient process for the preparation of the betanitriles is as follows:

Procedure B

The required methyl alkyl ketone (1 mol), cyanoacetic acid (93.5 g, 1.1 mol), ammonium acetate (13 g, 0.17 mol) and toluene (175 ml) were stirred under reflux (pot temperature 140°-160° C.) in a Dean-Stark apparatus until carbon dioxide ceased to be evolved (3-6 hours). The resultant mixture was cooled, washed with saturated aqueous sodium hydrogen carbonate (2×50 ml) and water (50 ml) then the solvent was removed under reduced pressure. The crude mixture of nitriles was then added to one quarter of its volume of 50% aqueous sodium hydroxide to which Tergitol* (3 drops) had been added. The resulting mixture was stirred under reflux for 1 hour then cooled. The organic layer was removed, washed with water (3×50 ml) and distilled. 5% Palladium on carbon (0.1% by weight relative to the nitrile mixture) was then added followed by ethyl acetate (2×weight of distillate) and the suspension stirred vigorously in an atmosphere of hydrogen until uptake of gas ceased. The catalyst was removed by filtration and the solvent by evaporation under reduced pressure. Fractional distillation of the residue afforded the desired 3-methyl substituted nitrile.

*Tergitol is a trade name for a surfactant (Union Carbide).

The following table sets out the physical and the organoleptic properties of the nitriles useful in this invention:

TABLE

Sample	Series	Carbon Chain Length	Name	Structure
1	α-methyl	8	2-methyloctanonitrile	$CH_3(CH_2)_5CHCH_3CH$
2	α-methyl	9	2-methylnonanonitrile	$CH_3(CH_2)_6CHCH_3CN$
3	α-methyl	10	2-methyldecanonitrile	$CH_3(CH_2)_7CHCH_3CN$
4	α-methyl	11	2-methylundecanonitrile	$CH_3(CH_2)_8CHCH_3CN$
5	α-methyl	12	2-methyldodecanonitrile	$CH_3(CH_2)_9CHCH_3CN$
6	β-methyl	8	3-methyloctanonitrile	$CH_3(CH_2)_4CHCH_3CH_2CN$
7	β-methyl	9	3-methylnonanonitrile	$CH_3(CH_2)_5CHCH_3CH_2CN$
8	β-methyl	10	3-methyldecanonitrile	$CH_3(CH_2)_6CHCH_3CH_2CN$
9	β-methyl	11	3-methylundecanonitrile	$CH_3(CH_2)_7CHCH_3CH_2CN$
10	β-methyl	12	3-methyldodecanonitrile	$CH_3(CH_2)_8CHCH_3CH_2CN$

Sample	Preparation	Boiling Point (lit. bp)	Odour Description
1	Procedure A, 76% yield from 2-octanone	78-80° C. at 8 m bar (85 at 10 mm Hg)	Floral jasminic character with some celery aspects and a hint of coconut/lactone - very diffusive.
2	Procedure A, 69% yield	72-73° C. at 3 m bar	Soft, floral, lactonic,

TABLE-continued

	from 2-nonanone	(100 at 10 mm Hg)	jasmine/peachy character.
3	Procedure A, 77% yield from 2-decanone	85–87° C. at 3 m bar (115 at 10 mm Hg)	A fine, light, jasmine/floral character with a soft peach quality.
4	Procedure A, 74% yield from 2-undecanone	84° C. at 1 m bar (133 at 12 mm Hg)	Fresh, floral with some lilac character - tenacious.
5	Procedure A, 59% yield from 2-dodecanone	125–127° C. at 7 m bar (146 at 10 mm Hg)	Soft, floral with a green jasminic type odour - very persistent.
6	Procedure B, 59% yield from 2-heptanone	66–68° C. at 4 m bar (207–8 at 760 mm Hg)	An unusual floral type consisting of a distinct fatty jasminic character combined with an agrumen quality.
7	Procedure B, 16% yield from 2-octanone	93° C. at 8 m bar (95–6 at 2–3 mm Hg)	Fresh, jasminic floral type with a slightly green quality.
8	Procedure B, 49% yield from 2-nonanone	72–74° C. at 0.7 m bar	Soft, citrus floral - reminiscent of jasmine.
9	Procedure B, 35% yield from 2-decanone	99–100° C. at 3 m bar	Light, fresh, green, floral suggesting lilac, with slight citrus undertones.
10	Procedure B, 26% yield from 2-undecanone	95–97° C. at 0.7 m bar	Distinct orange character which is suffused by a light green sea-fresh quality.

The following are two examples of perfume compositions comprising the nitriles of this invention:

Formula 1	
Phenylethyl Alcohol	30.5
Terpineol	6.0
Paratertiary butyl cyclohexyl acetate high cis (PPL)	15.0
Benzyl Salicylate	14.8
Cinnamic Alcohol	10.0
Sandalone (PPL)	5.0
Galaxolide (IFF)	3.0
Hexyl Cinnamic Aldehyde	10.0
Coumarin	2.0
Rose Base AB 380 (PPL)	2.0
Isoeugenol	0.1
Vetivert Brazilian	0.1
Nitrile No 3	1.5

Formula 1 in the absence of nitrile 3 has a floral, woody bouquet suitable for a toilet soap. The addition of 1.5% of nitrile 3 enhances the overall freshness, giving a light floral, fruity effect. Using the above formulation but substituting nitrile 9 in place of nitrile 3, a perfume is created having an added fresh lightness with an enhanced floral, fruity and citrus character.

The three novel nitriles provided by this invention are those numbered 8, 9 and 10 in the samples list and their mass spectral data are as follows.

Sample		Base Peak	M1	M2	M3	M4	M5
8	C_{10}	41	43:85	57:84	68:66	55:50	96:46
9	C_{11}	41	57:85	43:84	68:56	55:50	69:43
10	C_{12}	41	57:92	43:90	55:54	68:53	70:48

Perfumes formulated using as an odorous component the nitriles provided by this invention may be employed in the various products, such as soaps, detergents, hairsprays, talcum powders and the like, which are normally augmented by the addition of a perfume.

I claim:

1. A perfume composition comprising at least two perfume components and, in addition, as an odour providing component, an organoleptically discernible amount of a nitrile of the formula:

$$CH_3(CH_2)_nRCN$$

in which

R=—$CHCH_3$— or —$CHCH_3CH_2$— and in which, when

R=—$CHCH_3$—, n is an integer from 5–9 and when R=—$CHCH_3CH_2$—, n is an integer from 4–8,

the amount of the nitrile not exceeding 95% by weight of the perfume composition and the nitrile being characterized by its stability in the use or storage of said composition.

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