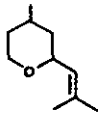
Dihydroroseoxide—A Unique New Aroma Chemical

By G. Schindler and F. Vogel, Application R + D, BASF AG, Ludwigshafen, West Germany

Rose oxides were isolated for the first time in 1959 from Bulgarian rose oil.[1] Shortly later it was discovered that this particular class of substances occurs generally in rose oils as well as in many plants of the Pelargonium family. Chemically, rose oxide (figure 1) is a substituted pyrane derivative of which four isomers have been found in nature.



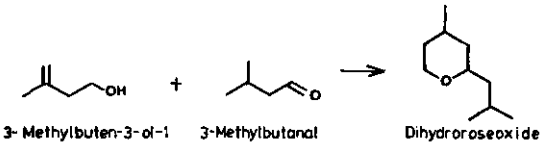
Roseoxide

Each of the four isomers has its particular odor characteristics. Their strong, powerful and irradiating odor has led to some use in specialty fragrances sometimes imparting dramatic effects into a perfume composition.

Today, however, rose oxides are still considered as a rare specialty as they suffer from several major drawbacks. They have a comparatively limited stability in mass market products like soap and detergents, they have a price limiting the applicability to a small range of fashion perfumes and they have limited availability.

Chemistry

The desirability of an affordable aroma chemical with the olfactory properties of rose oxides prompted us to study the synthesis of chemical analogues to which one might gain an easier access. As a result, a new synthetic aroma chemical named dihydroroseoxide has been synthesized from easily available starting materials and represents a cis/trans (70/30) mixture of 2-(2'-methylpropyl)-4-methyl-hydropyrane. The synthetic pathway is indicated in figure 2.



3-Methylbuten-3-ol-1 + 3-Methylbutanal → Dihydroroseoxide

Properties

The synthetic basis not only allows ample supply in constant quality but makes it possible to offer dihydroroseoxide at only one sixth the cost of some natural rose oxides.

Because of its structural similarity to the rose oxides, dihydroroseoxide has a very similar odor profile. It exhibits the typical geranium and rose notes, but is not afflicted with the aggressive phenolic gassy bynotes of natural rose oxides. It has a greater softness in addition to mild herbaceous-green and slightly metallic undertones. The odor tenacity of dihydroroseoxide is rather poor, similar to the rose oxides, being perceptible for about half an hour on the blotter strip.

The saturated structure of the product made it possible to overcome an important handicap of the nature identical product, namely insufficient stability. We found dihydroroseoxide to be stable between pH 4-10. It exhibits a high thermal stability as well as good stability in soaps and detergents. The saturated chemical structure leads to an excellent UV-stability so that no discoloration has been detected after light exposure.

Application

The superior stability of dihydroroseoxide opens exciting new areas of the perfumer for creative compounds in fine fragrances as well as mass market products. The synthetic origin guarantees not only an affordable price but also unlimited supply in constant quality. Dihydroroseoxide lends interesting effects to many perfume compositions, especially in rose, floral, lavender and lavandin accentuated notes along with a great variety of herbaceous and fancy accords. Its stability allows incorporation into soaps and detergents, shampoos and creams. It does not discolor in all these major consumer products, which is of obvious importance to the soap and detergent industry.

Dihydroroseoxide may be applied in a typical range of 0.5 percent, but it can be used even above 5 percent without deteriorating the intended basic odor character of a compound while still imparting power, deepness and irradiation to the composition. The highest dosage of dihydroroseoxide seems to be practicable in moderately priced lavender and lavandin notes as well as compounds of the fresh herbaceous-green family.

The two types (formulas 1 and 2) shown here may serve as a suggestion.

Dihydroroseoxide has been evaluated in toxicological tests according to the procedures of RIFM. The results indicate that the product is safe for use in fragrance products.[2]

The combination of the interesting odor profile of dihydroroseoxide with availability in larger quantities, superior stability and an attractive cost will broaden the scope of possibilities in fragrance compounding and will open up new routes to a wide range of notes in creative perfumery.

Formula 1. Rose Type

Citronellol	265
Phenylethylalcohol	235
Geraniol	120
Linalool	60
Phenylethylacetate	20
Benzylacetate	15
Farnesol	10
Dihydroroseoxide	5
Diethylphthalate	270
	1000

Formula 2. Lavender Type

Linalool	455
Linalylacetate	315
Ocimene	33
Eucalyptol	12
Borneol	15
Terpentine oil	15
Terpineol	10
Dihydroroseoxide	10
Diethylphthalate	135
	1000

Accompanying this text are three samples of materials. One is the pure dihydroroseoxide. The other two are demonstration accord 110-1 (without dihydroroseoxide) and demonstration accord 110-2 (with dihydroroseoxide). The formulas for these two accords are included on page 31. If the samples of materials are missing from this article, write for additional materials to Mr. Konrad Roser, MEF, BASF, D6700 Ludwigshafen, West Germany.

References

Address correspondence to Herr Dr. F. Vogel, BASF Aktiengesellschaft, D-6700 Ludwigshafen, West Germany.

1. C. F. Seidel and M. Stoll, Helv. Chim. Acta **42**, 1830, 1959.
2. Test results available on request

We have placed smelling samples in this article, in order to illustrate this article. Included is a sample of the pure material, and of two accords, one with and one without dihydroroseoxide. In this industry, we communicate with our noses and no pictures or words are even close to an adequate substitute for smelling.

We hope that you find this to be a most interesting and valuable addition to our editorial program. We would appreciate hearing from you on the following points:

1. Did the samples in this issue arrive in good condition without breaking or leaking?
2. Would you like to continue to get smelling samples of materials that are described in this magazine in the future?
3. If you have any further suggestions for development along this line, we would like very much to hear from you.

Stanley E. Allured
Publisher

Smelling Samples

Dihydroroseoxide

Accord 110-1

	Accord 110 - 1	Accord 110 - 2
Terpineol	15.0	15.0
p.tert.Butylcyclohexylacetate	5.0	5.0
Lilial (Givaudan)	5.0	5.0
Benzyl acetate	12.0	12.0
Geraniol	6.0	6.0
Cyclamen aldehyde	3.0	3.0
Veloutone (Firmenich)	0.5	0.5
Rose base (FDO)	12.5	12.5
Traseolide 70 (Naarden)	6.0	6.0
Citronellol	6.0	6.0
Cyclacet (IFF)	8.0	8.0
Benzyl benzoate	10.0	10.0
Lavandin oil	6.0	6.0
Aldehyde C14, 10%	1.0	1.0
Dihydroroseoxide	-	4.0
Diethylphtalate	4.0	-
	100.0	100.0

Accord 110-2

If the smelling samples referred to above have been removed from this publication before you receive it, contact the nearest office of BASF or Fritzsche, Dodge & Olcott, or write directly to Konrad Roser, MEF/MR-D205, BASF Aktiengesellschaft, D-6700 Ludwigshafen, West Germany.