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ANALYSIS OF BRAND NAME AND IMPOSTER FRAGRANCE FORMULATIONS

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Abstract

Refractometry and gas chromatography were used to study the relative compositions of a well known brand name fragrance and four imposter versions of the same fragrance. Results indicate that all imposter versions have a significantly lower refractive index than the brand name. Chromatography data reveals that none of the imposters are as complex in their formulation as the brand name. A comparison of the data indicates that a higher refractive index is correlated to a greater concentration of the components that create the base notes of the fragrance. This research suggests that a simple comparison of the refractive indices of multiple fragrances will provide a quick indication of how close their relative formulations are, and may be indicative of how long the fragrance will retain its scent.

Keywords: Fragrance, perfume, chromatography, refractive index

Introduction

A continuing research interest in our laboratory is the chemistry of consumer products, specifically in developing simple and inexpensive methods of analysis.

The global market for perfume products is influenced heavily by brand name products. In 2005, celebrity and celebrity endorsed brands represented 23 percent of the top 100 women's fragrances in the U.S. (1). Accordingly, many imposter versions have appeared on the market, and they typically sell at deep discounts.

To an experienced perfumer, the formulation of ingredients creates three layers, or notes (2,3). The top notes evaporate first, contributing to the initial scent. This scent fades quickly as the middle or heart notes become apparent, remaining for approximately 4 hours. Finally, the middle notes fade revealing the lower or base notes, which may last for up to 24 hours. Literature describes typical fragrances as being comprised of an alcohol and water base, which serves as the carrier for the ingredients that actually deliver the desired scent. It is generally understood that it is the identity, number of, and concentration of natural and synthetic ingredients that comprises the signature fragrance of a product. The exact formulations of successful fragrances are usually treated as trade secrets.

A literature search reveals work in this area and the analytical method of choice is typically GC-MS. For example, the difficulty of formulating an exact match of a fragrance when using GC-MS instrumentation has been noted (3). Mowery used imposter fragrances as the matrix for development of an undergraduate analytical experiment focusing on the capabilities of GC-MS instrumentation (4). The specific objective of our project was to use chromatography and refractometry to determine if there are measurable differences in the formulations of the brand name and imposter products presently being sold.

Experimental

The following materials were obtained for the development and validation of the method. A Fragrance Materials chromatography standard was obtained from the Restek Corporation (5). This standard contains 12 components commonly used in formulating fragrances. The ingredients in the mixture are listed in Table 1. In addition, 15 pure individual fragrance component standards were donated to the college from a local manufacturer of flavor and fragrance ingredients. The refractive indices for all components ranged from 1.3900 to 1.6190. They were used for the chromatographic method development and identification of perfume ingredients.

The brand name formulation in the research was "White Diamonds", a signature perfume from Elizabeth Taylor, available in retail stores or online (6). For comparison, 4 imposter versions of this fragrance were purchased from retail cosmetic and beauty stores in Burlington County, NJ.

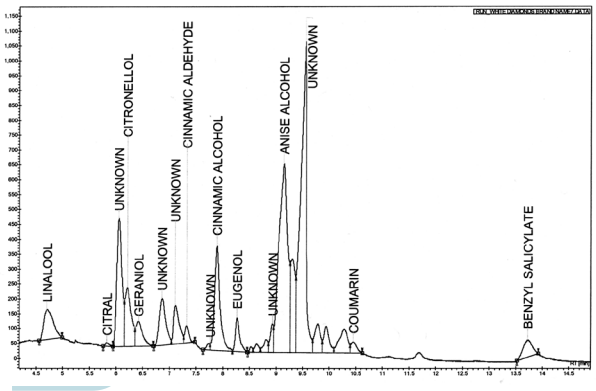

Figure 1. Brand Name White Diamonds Chromatogram. This fragrance had a refractive index of 1.3997 and 23 components integrating to a total of 19.81% of the total composition.

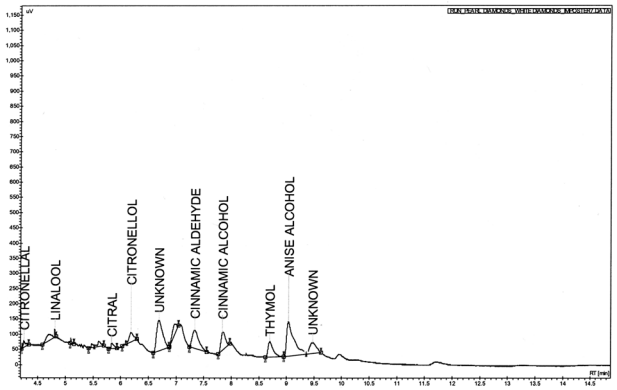

Figure 2. Imposter A Chromatogram. This fragrance had a refractive index of 1.3744 and 15 components integrating to 2.17% of the total composition.

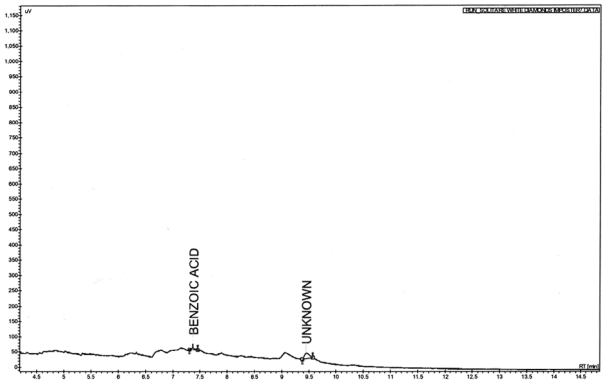

Figure 3. Imposter B Chromatogram. This fragrance had a refractive index of 1.3674 and 2 components integrating to 0.12% of the total composition.

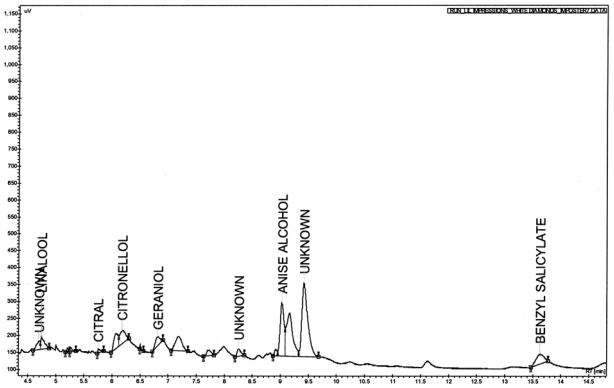

Figure 4. Imposter C Chromatogram. This fragrance had a refractive index of 1.3798 and 17 components integrating to 3.46% of the total composition.

Refractometry readings were measured on a Reichert Instrument Model Mark II Plus. Data represent an average of 5 trials and were corrected to 20^0C. Gas chromatography method used a Varian 3900 Model with a CP Wax 57 CB 25m x 0.53mm column. The oven temperature was started at 70^0C and ramped to 200^0C at a rate of 20^0C per minute and then held to 15 minutes. The detector was a TCD, sample size was 1.0 µL, and the carrier gas was helium. The identification of the components in the purchased fragrances was accomplished by spiking the analytes with the fragrance component standards. Additional details on the chromatographic method development, software, and reduction of data used in our lab have been previously published (7).

Safety

Alcohol based fragrances are typically flammable and should be handled accordingly. Some fragrances and fragrance components may create an allergic response in some individuals; therefore, inhalation and skin contact should be avoided by those individuals.

Results and Discussion

Refractive Index Results

As mentioned before, all fragrance components used in our study have refractive indices significantly higher than both ethanol (1.3611) and water (1.3331). Table 2 represents the refractive index data of the fragrances in our study. Imposters B and D have essentially the same refractive index, which is significantly lower than other samples. Imposters A and C have similar refractive indices, which are higher than imposters B and D, but significantly lower than the brand name.

Chromatography Results

Table 3 shows a summary of the chromatography results. The ethanol and water eluted at 0.7 minutes and 1.2 minutes respectively. The less volatile components eluted between 4 minutes and 15 minutes. Figures 1 through 5 are representative chromatograms of the fragrances showing greater resolution of the low

concentration components that would be lost if the chromatogram was scaled to include the complete ethanol peak. Inspection of the chromatograms coupled with the data in Table 3 illustrates the following trends. The brand name fragrance has the lowest combined concentration of ethanol and water and the greatest number and concentration of the less volatile components. There is an unidentified peak at about 9.5 minutes that integrates to 4.7% of the composition. Anecdotal evidence suggests that it could possibly be hydroxyisohexyl-3-cyclohexene carboxaldehyde, a commonly used fragrance ingredient, but we were not able to confirm the identity during this study because we did not have the standard. The peak at 13.7 minutes was identified as benzyl salicylate.

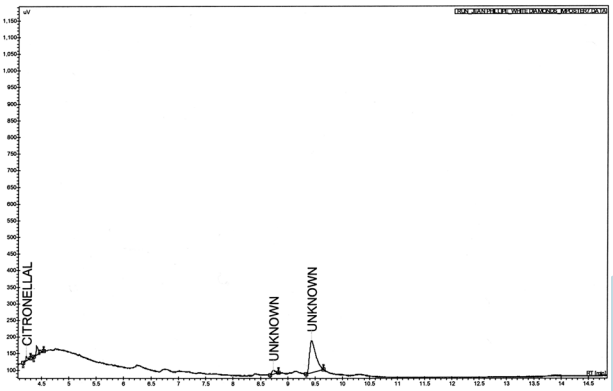

Figure 5. Imposter D Chromatogram. This fragrance had a refractive index of 1.3675 and 5 components integrating to 0.42% of the total composition.

Imposter A has a similar concentration of ethanol as the name brand, but significantly more water. Thus the number and concentration of the less volatile components is reduced. Imposter B contains greater than 99% ethanol and few of the less volatile components. Imposter C contains 96% ethanol and some of the same less volatile components as the brand name, including about 1% of the unidentified component at 9.5 minutes and also some benzyl salicylate. Imposter D contains a relatively low concentration of ethanol at 68% and high concentration of water at 31%. The unidentified component at 9.5 minutes is present.

In summary, when compared to the name brand, Imposters B and D have the lowest refractive indices and are comprised of essentially ethanol and water, with a few trace level components of lower volatility. Imposters A and C are closer in refractive index and contain some of the same components as the brand name, but are still measurably less complex.

Limitations

There were several fragrance components that we were not able to identify because we did not have the required standard nor did we have GC-MS capability.

Table 1. Fragrance Materials Association Mix Rtx-1701

COMPOUND	CAS #	REFRACTIVE INDEX
Ethyl Butyrate	105-54-4	1.3900^{20}
Limonene	5989-27-5	1.4710^{20}
Eucalyptol	470-82-6	1.4550^{20}
Geraniol	106-24-1	1.4690^{20}
Benzoic Acid	65-85-0	1.5640^{20}
Cinnamic Aldehyde	104-55-2	1.6190^{20}
Hydroxycitronellal	107-75-5	1.4350^{20}
Cinnamyl Alcohol	104-54-1	1.5120^{20}
Cinnamyl Acetate	103-54-8	1.5390^{20}
Vanillin	121-33-5	1.5370^{20}
Benzyl Salicylate	118-58-1	1.5680^{20}

Table 2. Refractive Index Data

Fragrance	RI*	Standard Deviation
White Diamonds	1.3997	0.0022
Imposter A	1.3744	0.0002
Imposter B	1.3674	0.0003
Imposter C	1.3798	0.0009
Imposter D	1.3675	0.0003

*Refractive Index corrected to 20°C mean of 5 trials

Table 3. Summary of Data from Chromatograms.

Figure	Fragrance	Ethanol % Area	Water % Area	Number of Integrated Peaks Eluting Between 4 and 15 Minutes	Total % Area of Peaks Eluting Between 4 and 15 Minutes
1	White Diamonds	75.49	4.62	23	19.81
2	Imposter A	82.32	15.08	15	2.17
3	Imposter B	99.37	0.41	2	0.12
4	Imposter C	95.53	0.39	17	3.46
5	Imposter D	67.54	31.33	5	0.42

We did not, as part of this work, develop calibration curves for each of the components. Therefore while the relative percentages are comparable across fragrances, the absolute accuracy of reported percentages can be improved. It is clear at this point in time, none of the imposters are as complex as the brand name, however manufacturers may change their formulations from time to time.

Conclusion

Our research suggests that a higher refractive index predicts a greater number of and/or concentration of fragrance ingredients, resulting in a more complex and longer lasting scent. How the chemistry differences in the fragrances manifest themselves into actual differences in scent is a subjective matter. The results of comparative smell tests conducted in our laboratory on these fragrances are available from the author by request.

Acknowledgments

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