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Additional Information

# **A sensory 3-D map of the odor description space derived from a comparison of numeric odor profile databases**

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## **ABSTRACT**

Many authors have proposed different schemes of odor classification, which are useful to aid the complex task of describing smells. However, reaching a consensus on a particular classification seems difficult because our psychophysical space of odor description is a continuum and is not clustered into well-defined categories. An alternative approach is to describe the perceptual space of odors as a low-dimensional coordinate system. This idea was first proposed by Crocker and Henderson in 1927, who suggested using numeric profiles based on four dimensions: “fragrant,” “acid,” “burnt,” and “caprylic.” In the present work, the odor profiles of 144 aroma chemicals were compared by means of statistical regression with comparable numeric odor profiles obtained from two databases, enabling a plausible interpretation of the four dimensions. Based on the results and taking into account comparable 2-D sensory maps of odor descriptors from the literature, a 3-D sensory map (Odor Cube) has been drawn up to improve understanding of the similarities and dissimilarities of the odor descriptors most frequently used in fragrance chemistry.

**Key words:** fragrance, odor character descriptor, psychophysics, sensory map

## INTRODUCTION

Since the Linnaean classification of odors nearly three centuries ago (Linnaeus 1756), many other schemes have been postulated (Table 1). The classification of smells implicitly assumes that the structure of an odor description space is determined by a discrete number of well-defined categories, yet this hypothesis has not been supported by experimental evidence. An alternative was put forward by the cosmetic chemists Crocker and Henderson, who were probably the first to describe odor perception as a low-dimensional coordinate space based on four references (“fragrant,” “acid,” “burnt,” and “caprylic”). Under this classification, any odor could be projected onto this space and described numerically with the coordinates or contributions of each of the four reference attributes (Crocker and Henderson 1927). In a subsequent work, an Odor Directory was compiled, containing the four-digit profiles of 244 aroma chemicals (Crocker and Dillon 1949).

### [TABLE 1 ABOUT HERE]

Crocker’s system was well received at the time (Boring 1928; Hazzard 1930), and the method yielded reasonable results (Dorough et al. 1941). However, it failed to give consistent results when used by untrained subjects (Ross and Harriman 1949). Moreover, it becomes confusing and subjective to try to characterize a given smell with a four-digit profile (Moncrieff 1966). Crocker and Henderson proposed a series of eight odorants as a reference for each attribute with a varying degree of applicability, but in practice, using these references is quite complicated.

The novelty of Crocker’s system at the time it was published has given its place in history (Harper et al. 1968a) and it has led to many studies that have compiled numeric odor profiles by rating smell similarity based on a series of reference odorants (Schutz 1964; Yoshida 1975; Boelens and Haring 1981). However, Crocker’s Odor Directory has not been re-analyzed yet. One of the main goals of this paper is to provide an appropriate interpretation of the four descriptive dimensions so as to explore what was, at the time, an influential approach to odor categorization.

Based on the results of the statistical analyses performed, a sensory three-dimensional (3-D) odor map was developed to reflect the similarities and dissimilarities between the odor descriptors commonly used in fragrance chemistry. The issue was how to project or “condense” Crocker’s four dimensions into just three axes. This 3-D odor map, called the Odor Cube, was based on the well-known Odor Prism (Henning 1916), and it was developed so that the projection over two axes was equivalent to the Odor Effects Diagram (Jellinek 1951), as this diagram is consistent with odor maps derived from consumer research (Thiboud 1991; Jellinek 1992; Richardson 1999), and is built on two meaningful dimensions (Zarzo and Stanton 2009).

In the opinion of Sell (2004), “currently there are no agreed universal standards of odor description, and apparent agreement can be misleading”. Thus, the proposed Odor Cube may constitute a valuable tool to aid the complex process of odor description and to improve verbal odor profiles. An accurate description is decisive for assessing the quality of foodstuffs and scented products. It is also a crucial step in the training of sensory panels as well as in consumer research.

## **MATERIALS AND METHODS**

### Description of the Odor Directory

The Odor Directory contains the four-digit profile of 244 aroma chemicals, 98 essential oils and another 19 natural materials. The four-digit description of 16 additional chemicals is also available (Harper et al. 1968a). The profiles were obtained experimentally by both authors (Crocker and Dillon 1949) and were designated as “odor numbers.” Each digit represents the perceived “intensity” of the reference attribute to the smell on a scale from 1 (very weak) to 8 (very strong).

### Comparison of odor profiles with the B-H database

In order to correctly analyze the information contained in the Odor Directory, two olfactory databases were considered. One of them, which will be referred to hereafter as the B-H database, is a broad compilation of numeric odor profiles obtained by a panel of six perfumers. The panel smelled 309 aroma chemicals and rated these odors’ similarity to 30 reference materials on a scale of 0-9 (Boelens and Haring 1981). Each reference was selected as a standard for a certain odor descriptor. The reference for “aromatic” was vanillin and, hence, this attribute was renamed as “vanilla” for the purposes of clarity.

It turns out that 144 aroma chemicals are contained both in the B-H database and the Odor Directory. Stepwise multiple linear regression was used to predict each of Crocker’s four attributes as a function of the 30 descriptors in the B-H database for these compounds. All the regression models were carried out using Statgraphics 5.1 software (Statpoint Technologies Inc., Warrenton VA). Compounds with unusual residuals were discarded.

### Comparison of odor profiles using Dravnieks’ Atlas

In our study, we also used Dravnieks’ Atlas, a database of numeric odor profiles made up of 146 descriptors for a set of 160 samples. A panel of 120-140 individuals smelled each sample and assigned for each term the score that best characterized the “degree of presence” of that odor in the sample on a scale of 0-5 (Dravnieks 1985).

A comparison of the list of materials in this Atlas and the Odor Directory revealed that there was an overlap between 47 aroma chemicals and six essential oils. Five additional odorants in the Atlas have analogous materials in the Odor Directory with a similar chemical structure and comparable odor, and they were also matched for the comparison. Stepwise regression was used to predict Crocker’s attributes according to the descriptors in the Atlas for the 58 materials which had available odor numbers.

### Construction of a 3-D descriptive model

Very few attempts have tried to represent odor descriptors in a 3-D space. The first serious approach was based on six reference odors located at the vertices of an Odor Prism (Henning 1916). Based on this idea, an Odor Cube was drawn up to graphically depict the relationships between perfumery descriptors. The cube’s development was based on the Odor Effects Diagram, a 2-D sensory map of odor descriptors in the shape of a square (Jellinek 1951) that has been validated experimentally (Zarzo and Stanton 2009). Adding a third dimension to this diagram leads to the creation of a cube. The aim was to properly place the main odor descriptors on the edges, vertices and faces of this cube so that their projection over the base of the cube should resemble Jellinek’s diagram as much as possible.

## OBSERVATIONS

### Effect of intensity

Odor numbers represent the perceived intensity of fragrant, acid, burnt, and caprylic odor characters. The term “intensity” used by Crocker and Dillon is misleading because it may indicate that the strong/weak smell of an odorant, which is independent of its odor character, may affect the reported odor numbers. Most related psychophysical studies try to avoid this effect by assessing samples at similar smell intensity (Amoore and Venstrom 1967; Dravnieks 1985). In order to study this issue, the odor strength (OS) of all compounds was retrieved from the Good Scents Company website ([www.thegoodscentscompany.com](http://www.thegoodscentscompany.com)) and was coded as shown below. This information was obtained for 244 of the 260 aroma chemicals with available odor numbers: two of them were odorless (OS=0), 14 were weak (OS=1), 186 were medium (OS=2), and 42 were strong odorants (OS=3). Multiple regression was applied to predict the odor strength based on the scores for acid, burnt and caprylic characters (Equation 1,  $R^2 = 0.28$ ).

$$OS = 1.19 + 0.057 \cdot S_{\text{acid}} + 0.066 \cdot S_{\text{burnt}} + 0.104 \cdot S_{\text{caprylic}} \quad (1)$$

The low  $p$ -values associated with regression coefficients, which will be called  $p_{rc}$ , indicate a statistically significant effect ( $p_{rc} \leq 0.001$ ). Thus, Crocker and Dillon tended to assign higher odor numbers to stronger odors, except maybe in the case of “fragrant.” In fact, the authors mention that caprylic=1 was assigned to materials with weak odors, which applies to three chemicals. These odor numbers were not reliable and, hence, they were disregarded for the rest of the study.

The information about OS has to be taken into account when trying to relate the four odor characters with descriptors from other databases. For this purpose, an indicator variable  $Z_{OS=3}$  was obtained that took the value 1 when OS=3 and zero when otherwise. It was considered as an explanatory variable in all of the regression models carried out. Given that multiple linear regression is not able to cope with missing values, OS=2 was assigned to the missing values of this parameter.

### Interpretation of “acid” in the Odor Directory

#### Prediction of “acid” using the B-H database

“Acid” yielded the highest correlation with “sourish,” “fruity” and “green.” These three variables enter in the predictive model (Equation 2:  $R^2 = 0.40$ ,  $p_{rc} < 0.008$ ,  $n = 142$ ) and their regression coefficients were similar, which implies that “acid” was interpreted as an intermediate odor character between these three descriptors. In reality, as the intensity of acid increases from 1 to 8, the odor is mildly fruity at first, then becomes citral-like, and finally is sharp and irritating (Crocker and Dillon 1949). The first principal component (PC1) of the B-H database differentiates between light vs. heavy (tenacious) odors and is basically defined by “fresh,” “sourish,” “green,” and “citrusy” (Zarzo 2013), which implies that “acid” can be interpreted analogously.

$$\text{acid} = 2.18 + 0.27 \cdot \text{sourish} + 0.29 \cdot \text{green} + 0.30 \cdot \text{fruity} + 0.80 \cdot Z_{OS=3} + 2.80 \cdot Z_{\text{spicy}>5} \quad (2)$$

The “sourish” quality of green and citrus odors is well known in perfumery. However, the correlation between “acid” and “citrusy” is not statistically significant ( $r = 0.15$ ,  $p = 0.08$ ) because the B-H database has very few citrus odorants in common with the Odor Directory.

Crocker's criterion of describing fruity odors as acid may be arguable because citrus and fruity (non-citrus) scents are usually regarded as independent categories (Table 1). Moreover, all but one of the 22 compounds in the B-H database described as fruity>5 (on a 0-9 scale) are slightly sour (sourish<5).

The variable  $Z_{OS=3}$  in Equation (2) implies, as stated above, that Crocker and Dillon assigned higher ratings on average to the strongest odorants.  $Z_{spicy>5}$  takes the value 1 for the five odorants with the highest spicy smell, which satisfy the condition spicy>5. Taking into account that all spicy fragrances share a common pungency and sharpness (Thiboud 1991), the effect of this variable suggests that "acid" was also interpreted as pungent, probably because carboxylic acids like acetic acid (3-8-0-3) have a sourish smell and produce a pungent (irritating) chemesthetic sensation.

Diacetyl was given high scores (5-7-7-8), possibly as a result of its strong and pungent odor. Its apparently burnt and caprylic character is arguable and, hence, it was discarded.

#### Prediction of "acid" using Dravnieks' Atlas

Consistent results were obtained from Dravnieks' Atlas (Equation 3,  $R^2 = 0.43$ ,  $n = 58$ ). The variables in this model and the previous one (Equation 2) are basically equivalent. On one hand, the t[6] latent variable was obtained by applying Principal Component Analysis (PCA) to the Atlas. This contains the projections of odorants over the sixth principal component (PC6), which is basically defined by fruity descriptors. On the other hand, "fresh\_green\_vegetables" and "citrus+sour\_vinegar" obviously correspond to "green" and "sourish," respectively.

$$\text{acid} = 2.62 + 0.55 \cdot \text{fresh\_green\_vegs} + 0.35 \cdot \text{t}[6] + 0.039 \cdot (\text{citrus+sour\_vinegar}) + 0.071 \cdot \text{spicy} \quad (3)$$

#### **Interpretation of "burnt" in the Odor Directory**

Crocker and Dillon interpreted "burnt" as "empyreumatic". This odor category was introduced long ago, giving toasted bread and roasted coffee as examples (von Haller 1763). The terms empyreumatic and pyrogenous refer to odors ranging from baked bread on one hand to wood tar, on the other (Harper et al. 1968a). An example of the latter is cade oil, which is described as burnt=8 due to its intense tar-like smell. This material was the reference for "smoky" in the B-H database. Obviously, "burnt" and "smoky" are related concepts.

#### Prediction of "burnt" using the B-H database

A sensory experiment found that "burnt" is well understood in odor descriptions, and includes two main types: toast and wood (pleasant), and burnt (unpleasant) (Harper et al. 1968b). Similarly, Crocker and Dillon considered that "burnt" determines woodiness in an odor but that in the highest ranges this reaches "empyreumatic." The presence of "woody" in Equation (4) is consistent with this interpretation ( $R^2 = 0.34$ ,  $p_{rc} < 0.02$ ,  $n = 140$ ). This equation was obtained after trying several alternatives and discarding two outliers. The presence of  $Z_{OS=3}$  again indicates that stronger odorants were rated with higher odor numbers.

$$\text{burnt} = 2.11 + 1.13 \cdot Z_{OS=3} + 0.20 \cdot \text{woody} + 0.13 \cdot \text{spicy} + 0.43 \cdot \text{tart\_dry} \quad (4)$$

The similarity between "smoky" and "woody" is well known in fragrance chemistry (Rowe 2000), and both variables are correlated in the B-H database ( $r = 0.29$ ). The reason seems to be that smoky odorants in perfumery evoke burning wood (bonfires) and, to a lesser extent, coal and stale cigarettes. However, the effect of "smoky" is not relevant in Equation

(4) ( $p = 0.2$ ) because only four compounds are described as smoky>1 out of the 144 chemicals shared by the B-H database and the Odor Directory.

The presence of “spicy” was unexpected. The reason seems to be that the reference material (eugenol) has a warm, clove-like, somewhat woody scent, which is similar to some empyreumatic odors like toasted bread. Strangely, “burnt” yielded the highest correlation with “tart\_dry” ( $r = 0.36$ ) and, hence, it appears in Equation (4). The reason could be that the reference material for “tart\_dry” (galbanum resinoid) smells somewhat spicy-woody, and both descriptors are contained in the model.

Phenol has a sickeningly sweet and tarry smell and, hence, phenolic odors may also be included in this empyreumatic class (Jaubert et al. 1995). In fact, guaiacol smells like phenol and some authors have regarded it as a standard for “burnt” (Schutz 1964; Harper 1975). Different studies have found a similarity between “phenolic” and “medicinal” (Harper et al. 1968c; Chastrette et al. 1988; Abe et al. 1990). The odor description of all compounds rated as burnt>5 was checked and, interestingly, most of them smelled phenolic or medicinal. Moreover, “smoky” and “medicinal” are correlated ( $r = 0.34$ ) in the B-H database. However, “medicinal” does not appear in Equation (4) ( $p = 0.1$ ), probably because its reference material (methyl salicylate) smells slightly burnt (8-2-2-3). It seems that the B-H database does not contain enough information to properly reflect empyreumatic odors.

#### Prediction of “burnt” using Dravnieks’ Atlas

“Burnt” is correlated with related descriptors in the Atlas, but also with “oak wood” ( $r = 0.33$ ), “almond” ( $r = 0.35$ ), and “nutty” ( $r = 0.26$ ). The resulting model (Equation 5:  $R^2 = 0.61$ ,  $p_{rc} \leq 0.0002$ ,  $n = 58$ ) is consistent with Crocker’s interpretation of “burnt”, and also with a recent analysis of Dravnieks’ Atlas that obtained 10 factors, one of which was determined by “popcorn” (a toasted odor), “burnt\_smoky,” nutty odors (peanut butter, almond), “woody,” etc. (Castro et al. 2013). Similar results were reported by another study using the same set of 146 descriptors (Jeltema and Southwick 1986).

$$\text{burnt} = 2.31 + 1.08 \cdot \text{burnt\_rubber} + 0.085 \cdot \text{almond} + 0.046 \cdot (\text{clove} + \text{cedarwood}) - 0.078 \cdot Z_{\text{leather}>2} \cdot (\text{almond} + \text{clove} + \text{cedarwood}) \quad (5)$$

The presence of “burnt\_rubber” makes sense, though it is probably not the best example of an empyreumatic smell. Taking into account that cedarwood oil and eugenol (clove-like) were the references for “woody” and “spicy” respectively in the B-H database, the sum clove+cedarwood is equivalent to the descriptors “woody” and “spicy” in Equation (4). Toasted odors are probably well represented by this variable. Some other descriptors in the Atlas are related to toasted, but the stepwise regression did not take them into consideration.

Another study found that “pyrogenous” yielded the highest similarity with “almond” (Chastrette et al. 1991), which ties in with the presence of the latter in Equation (5). Nut-like and woody odors are similar (Klein 1947), and they are often mapped close to “smoky” (Zarzo and Stanton 2009). Benzaldehyde is frequently considered as the reference for “almond” (Harper 1975; Jennings-White 1984). Untrained individuals would probably disagree in describing this odorant as burnt=8, unless they are instructed that “burnt” is used in a broad sense, covering smoky, toasted, grilled, woody, and nutty scents.

“Leather” is applied in perfumery to the smoky-animalic odors that are characteristic of the ingredients used in the leather tanning process, which justifies the correlation with “burnt” ( $r = 0.25$ ,  $p = 0.06$ ). However, if this descriptor is introduced directly into the model, its regression coefficient becomes negative due to an interaction with other variables. In order to facilitate an easier interpretation, an indicator variable  $Z_{\text{leather}>2}$  was created that took the value 1 for the 15 compounds satisfying the condition  $\text{leather}>2$ . The effect of “almond,” “clove” and “cedarwood” is cancelled out in Equation (5) for these odorants, and only their additional burnt-rubber character is taken into consideration.

### Interpretation of “caprylic” in the Odor Directory

The term “caprylic” comes from the Latin *capra* (goat) and it refers to a general class of often unpleasant smells, associated with various animals, sweat, urine and excreta (Harper et al. 1968b). The typical goat-like odor is exemplified by hexanoic acid (caproic acid), which is described as sour, fatty, sweat, and cheese-like. This odor class, first proposed by Linnaeus (1756), was made up of goaty, cheese, sweaty, and chestnut odors (Zwaardemaker 1925). Accordingly, the highest caprylic (c) scores were assigned by Crocker and Dillon to fecal-animalic (c=8) and fatty-rancid odors (c=7). However, high ratings were also assigned to bitter-herb materials (c=7) and minty/camphoraceous odors (c=6), which may be arguable. Thus, “caprylic” was used in a broad sense, and was not only restricted to odors resembling caproic acid.

The model obtained with the B-H database yielded a moderate goodness-of-fit (Equation 6:  $R^2 = 0.49$ ,  $p_{rc} < 0.006$ ,  $n = 142$ ). A higher value would probably have been obtained if hexanoic acid had been used as a reference in the B-H database.

$$\begin{aligned} \text{caprylic} = & 4.38 + 1.41 \cdot Z_{\text{OS}=3} + 0.28 \cdot \text{animal} + 0.20 \cdot (\text{fatty} + \text{aldehyde}) \\ & + 0.35 \cdot \text{tart\_dry} - 0.15 \cdot (\text{floral} + \text{citrusy} + \text{sourish}) \end{aligned} \quad (6)$$

For Dravnieks’ Atlas, Equation (7) was obtained with just three descriptors ( $R^2 = 0.58$ ,  $p_{rc} < 0.003$ ,  $n = 58$ ). Equation (8) is very similar ( $R^2 = 0.57$ ) given that “putrid” and “fecal” are related. The sum of floral+citrus is slightly significant ( $p = 0.05$ ), but the remaining variables are clearly relevant ( $p < 0.003$ ). The presence of  $Z_{\text{OS}=3}$  indicates once again that higher ratings were assigned to the strongest odorants.

$$\text{caprylic} = 3.31 + 0.98 \cdot Z_{\text{OS}=3} + 0.19 \cdot \text{putrid} + 0.21 \cdot (\text{alcoholic} + \text{bitter}) \quad (7)$$

$$\begin{aligned} \text{caprylic} = & 3.64 + 1.02 \cdot Z_{\text{OS}=3} + 0.20 \cdot \text{fecal} + 0.21 \cdot \text{alcoholic} \\ & + 0.10 \cdot \text{oily\_fatty} - 0.019 \cdot (\text{floral} + \text{citrus}) \end{aligned} \quad (8)$$

Strongly unpleasant animalic odors were described as caprylic=8, which justifies the presence of “animal,” “putrid” and “fecal” in Equations (6) - (8). In the Atlas, “caprylic” yields the highest correlation with “sickening” and “putrid,” and out of the 29 descriptors that had the highest correlation with “caprylic,” six of them corresponded to animalic odors (wet dog, sweaty, dirty linen, cadaverous, fecal, and sperm-like). A recent analysis of Dravnieks’ Atlas has found a factor determined by “putrid,” “sweaty,” “rancid,” and “fecal” (Castro et al. 2013), which clearly fits with the interpretation of “caprylic”.

Caprylic and ambrosial (erogenic) odors are related, though they are often regarded as independent categories (Table 1). In fact, ambergris and costus oil were described as caprylic=8, and a mixture of them was the reference material in the B-H database for



“erogenic”, which is correlated with “animal” ( $r = 0.46$ ). “Erogenic” and “citrus/sourish” are dissimilar odors (Zarzo and Stanton 2009), which ties in with the negative regression coefficient of the latter in Equations (6) and (8). The same criterion was adopted by Crocker and Dillon with citrus scents being rated as caprylic=3. Lower scores (caprylic=2) were assigned to floral scents, which is also reflected by Equations (6) and (8).

Given the fatty odor character of caproic acid, aldehydes and fatty alcohols were described as caprylic=7. “Fatty” and “aldehyde” are correlated in the B-H database ( $r = 0.56$ ) because their respective reference materials smell alike. Thus, it would seem more suitable to use their average (or sum, which is equivalent) for interpretation purposes. Hence, it is very interesting to find fatty+aldehyde in Equation (6) and “oily\_fatty” in Equation (8).

Crocker and Dillon assigned caprylic=7 to bitter-herb odorants like galbanum. This material was the reference for “tart\_dry” in the B-H database, which would explain the presence of this descriptor in Equation (6) and “bitter” in Equation (7). The only possible explanation is that bitter (non-sweet) herbal scents are typically found in agrestic areas, and farm-like (caprylic) smells are often associated with these areas. “Rustic” was actually proposed as a category of smells made up of herbaceous, lavender, minty, camphoraceous, green, earthy, and vegetable odors (Billot 1948). It is debatable whether to consider bitter herbal scents as highly caprylic because they are different to fatty, rancid, sweaty, or animalic odors, unless “caprylic” is understood in the broad sense of farm-like and agrestic smells.

Many herbs from rural areas exhibit camphoraceous and mentholic notes like rosemary, lavender, marjoram, etc. Perhaps this is why perfumery materials in which these notes predominate were described by Crocker and Dillon as caprylic=6, but this criterion is doubtful. Camphor-like notes are perceived as being somewhat chemical, which would explain the correlation between “caprylic” and “chemical” ( $r = 0.53$ ) as well as the presence of “alcoholic” in Equations (7) and (8) because this refers to chemical odors.

## **Interpretation of “fragrant” in the Odor Directory**

### Prediction of “fragrant” using the B-H database

The regression model for “fragrant” has a poor goodness-of-fit (Equation 9,  $R^2 = 0.18$ ,  $p_{rc} < 0.009$ ,  $n = 142$ ). The sum of “fatty” and “aldehyde” led to better results because they are related descriptors in the B-H database. This was also true in the case of “fresh” / “citrusy” and “vanilla” / “sweet.”

$$\text{fragrant} = 4.95 + 0.44 \cdot \text{erogenic} - 0.13 \cdot (\text{fatty} + \text{aldehyde}) + 0.11 \cdot (\text{fresh} + \text{citrusy}) + 0.10 \cdot (\text{vanilla} + \text{sweet}) \quad (9)$$

Crocker and Dillon assigned the highest “fragrance” intensities to heavy (tenacious) and even cloying (very sweet) materials. Accordingly, “vanilla+sweet” appear in Equation (9) and it was checked that most aroma chemicals that were rated as fragrant=8 smelled sweet. These scents, as well as erogenic and fresh/citrus odors, are pleasant and frequently found in commercial fragrances. Conversely, fatty and aldehydic odors are unpleasant, which ties in with the negative regression coefficient.

### Prediction of “fragrant” using Dravnieks’ Atlas

The “fragrant” descriptor of the Odor Directory ( $\text{frag}_{OD}$ ) is correlated with “fragrant” in the Atlas ( $r = 0.48$ ,  $p = 0.0001$ ), but  $\text{frag}_{OD}$  yielded a stronger correlation in absolute value

with “gasoline\_solvent” ( $r = -0.50$ ) and “aromatic” ( $r = 0.49$ ). Hence, both descriptors fit in the model (Equation 10,  $R^2 = 0.57$ ,  $n = 58$ ). Given that “aromatic” can be interpreted differently, Equation (11) was obtained ( $R^2 = 0.64$ ) by replacing this descriptor with “warm” and “cooling+citrus”.

$$\text{fragrant} = 4.55 + 0.52 \cdot Z_{\text{OS}=3} + 0.051 \cdot \text{aromatic} + 1.35 \cdot Z_{\text{s\_meat}>1} - 0.11 \cdot (\text{gasoline} + \text{metallic}) \quad (10)$$

$$\text{fragrant} = 4.14 + 0.65 \cdot Z_{\text{OS}=3} + 0.11 \cdot \text{warm} + 0.036 \cdot (\text{cooling} + \text{citrus}) + 1.34 \cdot Z_{\text{s\_meat}>1} - 0.11 \cdot (\text{gasoline} + \text{metallic}) \quad (11)$$

“Erogenic” and “powdery” are correlated in the B-H database ( $r = 0.49$ ). The reference materials for the latter smell warm (Zarzo & Stanton 2009). Thus, the effect of “erogenic” in Equation (9) can be interpreted as “warm” in Equation (11). The indicator variable  $Z_{\text{s\_meat}>1}$  takes the value 1 for the seven compounds that satisfy “seasoning for meat”  $> 1$ , which accounts for spicy odors. Warm, cool (refreshing), citrus and spicy scents are very typical in fragrances, which ties in with their positive coefficient in Equation (11).

“Gasoline\_solvent” and “metallic” were added because both are correlated and refer to odors perceived as chemical, artificial, and not present in nature. The negative coefficient of gasoline+metallic indicates that chemical odors decrease the perceived fragrant character. These odors are usually absent from commercial perfumes. If “gasoline+metallic” is discarded from Equation (10), the  $R^2$  decreases dramatically from 0.57 to 0.38. The B-H database does not contain any “chemical” descriptors, which would explain the low  $R^2$  of Equation (9).

The Linnaean odor classification system classed floral and balsamic odors as part of the “fragrant” category (Linnaeus 1756). The same criterion was adopted by Zwaardemaker (1925). Curiously, just a few years later, Crocker and Henderson (1927) seemed to interpret “fragrant” differently, because the effect of “floral” was neither significant in Equation (9) ( $p = 0.11$ ) nor in Equation (11) ( $p = 0.7$ ). The models obtained seem to indicate that “fragrant” was understood as the pleasant scents typically encountered in fragrances both for men and women.

### **A proposed 3-D map of the odor description space**

Henning’s famous Odor Prism, which was based on six reference categories, was probably the first serious attempt to describe odor space in three dimensions (Henning 1916). Based on this prism and after considering many alternative positions, an Odor Cube was proposed (Figure 1) reflecting the relationships between descriptors revealed by the statistical analyses carried out. Odor descriptors close to each other are supposed to be similar, which implies that they are likely to be encountered simultaneously in the verbal description of a given smell. Conversely, attributes located on opposite sides of the Odor Cube or which are far apart will rarely be applied together.

Crocker’s four attributes and related odors are precisely identified in the cube (gray regions in Figure 1). Descriptors that are supposed to be intermediate of two categories are placed in-between.

- “Acid” was located at one corner of the Odor Cube, and is close to similar odors like “sourish/citrus,” “green,” “fruity,” “tart,” and “sourish.” Pungent (irritating) is a tactile

perception related to acid. The proximity between “fruity” and “floral” is well known in perfumery.

- “Burnt” appears in another corner. The empyreumatic region is defined by “toasted,” “leather,” “nutty,” “woody,” and smoky odors like fresh tobacco smoke and roasted coffee. The proximity between “leather” and “civet” is interesting. “Clove” (spicy) was placed nearby because it is included in Equations (4) and (5). “Tart\_dry” was located between “acid” and “burnt,” which makes sense because it appears in Equation (4).

- “Caprylic” is depicted at one of the bottom corners. “Cheesy” and “sweaty” are related descriptors which are plotted very close by. Caprylic=8 corresponded to animalic odors, shown in the cube through “fecal/civet.” This term is placed near “earthy” because both evoke decomposition. Caprylic=7 was applied to fatty odors, which are also located in the caprylic region at the base of Figure 1. Thirdly, caprylic=6 and =5 was assigned to camphor-like and earthy odors, respectively, which is also reflected in the cube. Finally, the lowest ratings correspond to floral/citrus odors, which are placed on the opposite side. “Musk” and “animal” are related and, hence, the former was located close to the caprylic region together with “ambergris” (erogenic scents).

- “Fragrant” was regarded as a region on the cube which was determined by “powdery” (warm), “musk,” “floral,” and sweet-balsamic descriptors. This region is consistent with Equations (9) and (11). Spicy odors also increased the fragrant character (Equation 10), which ties in with the position of “cinnamon” in this region and “clove” nearby. Conversely, fatty and chemical odors decrease the fragrant perception (Equations 9-11) as does “putrid,” which is reflected in the opposite position of these descriptors. “Anise” was also included in the fragrant region given its sweet character, but other alternative positions may also be valid.

### **[FIGURE 1 ABOUT HERE]**

Figure 2 shows the orthogonal projection of descriptors in Figure 1 onto the base. The Odor Effect Diagram (Jellinek 1951) is depicted for comparison purposes, and also the position of descriptors derived from the PCA analysis of the B-H database (Zarzo and Stanton 2009). Their equivalent positions are worth noting. Jellinek’s diagram places fatty/rancid odors close to the “animal” descriptor, whilst conversely, “fatty” and “aldehyde” were regarded in the B-H database as antierogenic because their reference materials smell somewhat refreshing. The Odor Cube reconciles both criteria by placing “fatty” at the center. The Odor Effects diagram has been validated experimentally (for a review, see Zarzo and Stanton 2009), which supports the use of Odor Cube as a tool to better understand the relationships between perfumery descriptors.

### **[FIGURE 2 ABOUT HERE]**

Jellinek’s diagram is based on two orthogonal dimensions, one of which differentiates between antierogenic (refreshing) and erogenic odors (Figure 3A). However, an analysis of the B-H database has revealed that “powdery/warm” odors are also dissimilar to “cool/fresh.” This is depicted in Figure 3A as two dimensions opposite to cool scents, but which coincide in their projection on the cube base. The orthogonal dimension was “sweet” vs. “bitter” (Jellinek 1951), but it would seem more advisable to regard this polarity as a rotated latent structure based on Figure 1 and previous studies (Zarzo 2013).

The second principal component (PC2) of the B-H database was determined by “floral” vs. “earthy” (Figure 3A). This dimension could also be interpreted as “feminine” vs. “masculine” or even as “pleasant” vs. “unpleasant” (hedonic dimension), given that the most unpleasant smells are located around the putrid corner of the cube. Conversely, “sweet” is at the opposite corner, and nearby descriptors correspond to clearly pleasant scents. Finally, “chemical” vs. “fragrant” could also be considered as another polarity given that chemical notes decrease the fragrant perception, as discussed above.

In summary, understanding the underlying dimensions of the odor description space becomes difficult because they are not orthogonal (Figure 3A), an issue which psychophysical researchers have puzzled over for decades in terms of how to obtain 3-D odor maps.

### [FIGURE 3 ABOUT HERE]

Regarding the 10 factors deduced from the multivariate analysis of Dravnieks’ Atlas (Castro et al. 2013), the first two basically correspond to typically feminine and masculine scents, respectively, and can be approximately matched with the “floral” vs. “earthy” polarity in Figure 3A. Sweet-balsamic, fruity, citrus, empyreumatic, chemical, minty/camphor, and caprylic odors correspond to independent factors, something which is appropriately reflected by the Odor Cube. Another factor determined by “garlic\_onion”, “sulfidic”, and “putrid” corresponds to the “alliaceous” (garlic-like) odor class considered by several authors (Table 1). This odor character is seen to be in between “vegetable” and “sulfidic” odors (Figure 1). Some putrid products like rotten eggs smell sulfidic due to the presence of molecules containing sulfur. In fact, H<sub>2</sub>S was considered by Henning as a reference material for “putrid” (Gamble 1921).

### Discussion of the Odor Cube based on similar approaches

Very few 3-D sensory maps of odor descriptors have been proposed. Henning’s prism assumes six fundamental odors located at the vertices of a triangular prism with five faces (Figure 3B). It was built out from the descriptions given by a sensory panel about 466 odorous materials. Any odor was considered as a mixture, located on the surfaces and edges. Although it was possibly the first 3-D odor map ever proposed, it is uncertain how to locate a given odorant on this prism (Findley 1924). Because of this, it was argued that Henning’s proposed arrangement could be verified only in the broadest possible terms, but not in detail (MacDonald 1922; Dimmick 1922; 1927). Nonetheless, most of Henning’s six classes can be directly matched with the major descriptors in the Odor Cube (white circles in Figure 3), except in the case of “resinous”. The approximate position of frankincense (olibanum), which was the reference for this class, was based on Figure 2.

The Field of Odors is an olfactory representation created as a result of the statistical analysis of a large olfactory database (Jaubert et al. 1995). This odor map was based on six poles, four of which (citrus, sweet, pyrogenous, and sulfidic) can be directly matched with the Odor Cube. Another pole, “amine” (fishy-urinous odors) does not have a direct match. The sixth pole was “terpenic,” exemplified by  $\alpha$ -pinene (piney odor). Interestingly, “piney” could be matched with “resinous” in Henning’s prism. It seems that neither of the representations take into account the animalic/erogenic odors as a well-defined category, although this is very important in fragrance chemistry.

Another 3-D descriptive odor space was obtained by applying factor analysis to 83 numeric odor profiles (Paukner 1965). One dimension measured freshness and aggressiveness (green/sourish odor character) and reflected the light *vs.* heavy polarity, which is equivalent to PC1 in the B-H database (Zarzo 2013). Another orthogonal dimension called “evaluation” basically reflected the floral/fruity *vs.* burnt polarity of Henning’s prism, which corresponds to PC2 in the B-H database. The third axis called “activity”, differentiated “putrid” from the other odor classes. In fact, this category is located away from the others on the Odor Cube, which indicates that the 3-D odor description space obtained by Paukner has a reasonable analogy with the Odor Cube.

## CONCLUSION

Many classifications of odors are available in the literature (Table 1), but the verbal description of smells is a complex task because our olfactory descriptive space is highly dimensional. A pioneering approach proposed by Crocker and Henderson (1927) was to describe odors numerically based on four reference attributes (“fragrant,” “acid,” “burnt,” and “caprylic”). This method, which is of interest from a historical perspective, has been discussed here in detail.

The regression analyses performed to predict each of Crocker’s attributes as a function of descriptors in the other two databases revealed that it is very important to understand the interpretation of these attributes. For example, “acid” was applied to sourish and tart scents like lemon (citrusy) and vinegar, but also to refreshing (cool), green and fruity smells. “Burnt” was used in the sense of empyreumatic, comprising smoky, tarry, toasted, leathery, woody, nutty, and phenolic odors. “Caprylic” referred to farm-like animalic odors resembling hexanoic acid, some of which smell fecal, fatty or rancid (unpleasant), but it was also used for agrestic smells (bitter herbs) that are typical of rural areas. Finally, it seems that “fragrant” was applied to pleasant scents which were not perceived as having a chemical character, such as those frequently encountered in commercial fragrances for both men and women.

The equations obtained have shown that Crocker’s attributes can be predicted with a goodness-of-fit of about 40%-60%. Thus, with appropriate training, a sensory panel would be able to obtain reproducible four-digit profiles, albeit with low precision. Unexpectedly, it was found that Crocker’s profiles were affected by odor strength, which generates confusion because odor character and intensity are usually considered as two separate aspects of olfactory perception.

In recent decades, the application of statistical methods to olfactory databases has provided a quantitative way to map the relationships between odor descriptors (Abe et al. 1990; Chastrette et al. 1991; Jaubert et al. 1995; Zarzo and Stanton 2009; Castro et al. 2013). However, despite better understanding of the multivariate structure of our olfactory description space, attempts to reduce this space to a few dimensions are by no means easy.

Based on Henning’s Odor Prism, a similar 3-D representation with the shape of a cube is proposed here to illustrate the odor relationships that Crocker and Dillon had in mind when describing aroma chemicals. The four basic attributes and similar descriptors were suitably located on the Odor Cube according to the relationships reflected by Equations (2) - (11). An important property of this Cube is that the projection of descriptors onto the base is consistent with the Odor Effects Diagram (Jellinek 1951), with a sensory map obtained from the B-H database (Zarzo and Stanton 2009), with the Fragrance Wheel (Edwards 2010), and with 2-D

odor maps generated from consumer research (Thiboud 1991; Jellinek 1992; Richardson 1999).

Considering that describing a given smell is a complex task, the Odor Cube intends to facilitate verbal descriptions of aroma chemicals, particularly for untrained subjects, because it visually reflects the similarities and dissimilarities between common odor attributes. More accurate and reproducible odor profiles will obviously be obtained if sensory panels are trained with this kind of sensory maps. Nevertheless, it should be pointed out that the proposed Odor Cube is targeted at the field of fragrance chemistry and, hence, many food flavors like buttery or fishy smells are not properly represented.

## REFERENCES

- Abe H, Kanaya S, Komukai T, Takahashi Y, Sasaki S. 1990. Systemization of semantic descriptions of odors. *Anal Chim Acta*. 239:73-85.
- Amoore JE. 1962. The stereochemical theory of olfaction. I. Identification of seven primary odors. *Proc Sci Sect Toilet Goods Assoc*. 37(suppl.):1-13.
- Amoore JE, Venstrom D. 1967. Correlations between stereochemical assessments and organoleptic analysis of odorous compounds. In: Hayashi T, editor. *Olfaction and Taste II*. Oxford: Pergamon Press. p. 3-17.
- Bain A. 1855. *The Senses and the Intellect*. London: Parker.
- Bienfang RD. 1941. Dimensional characterisation of odors. *Chronica Bot*. 6:249-250.
- Billot M. 1948. Classification des odeurs. *Ind Parfum*. 3:87-92.
- Boelens H, Haring HG. 1981. *Molecular Structure and Olfactive Quality*. Bussum, The Netherlands: Internal Report Naarden International.
- Boring EG. 1928. A new system for the classification of odors. *Am J Psychol*. 40(2):345-349.
- Calkin RR, Jellinek JS. 1994. *Perfumery: Practice and Principles* (1st ed.). New York: Wiley.
- Castro JB, Ramanathan A, Chennubhotla CS. 2013. Categorical dimensions of human odor descriptor space revealed by non-negative matrix factorization. *PLoS One*. 8(9):e73289.
- Chastrette M, Elmouaffek A, Sauvegrain P. 1988. A multidimensional statistical study of similarities between 74 notes used in perfumery. *Chem Senses*. 13(2):295-305.
- Chastrette M., de Saint Laumer JY, Sauvegrain P. 1991. Analysis of a system of description of odors by means of four different multivariate statistical methods. *Chem Senses*. 16(1):81-93.
- Crocker EC, Dillon FN. 1949. Odor directory. *Am Perf Essent Oil Rev*. 53:297-301, 396-400.
- Crocker EC, Henderson LF. 1927. Analysis and classification of odors: an effort to develop a workable method. *Am Perf Essent Oil Rev*. 22:325-356.
- Dimmick FL. 1922. A note on Henning's smell series. *J Psychol*. 33(3):423-425.
- Dimmick FL. 1927. The investigation of olfactory qualities. *Psychol Rev*. 34(5):321-335.
- Dorough GL, Glass HB, Gresham TL, Malone GB, Reid EE. 1941. Structure-property relationships in some isomeric octanols. *J Am Chem Soc*. 63(11):3100-3110.
- Dravnieks A. 1985. *Atlas of Odor Character Profiles, Data Series DS 61*. Philadelphia PA: American Society for Testing and Materials.
- Edwards M. 2010. *Fragrances of the World: Parfums du Monde 2010* (26th ed.). Sydney: Fragrances of the World.
- Findley AE. 1924. Further studies on Henning's system of olfactory qualities. *Am J Psychol*. 35(3):436-445.

- Gamble EAM. 1921. Book review: *Der Geruch* by Henning H (1916). *Am J Psychol.* 32(2):290-295.
- Harper R. 1975. Some chemicals representing particular odor qualities. *Chem Sens Flav.* 1(3):353-357.
- Harper R, Bate-Smith EC, Land DG. 1968a. Odor Description and Odor Classification: A Multidisciplinary Examination. New York NY: Elsevier. p. 30-32, 82.
- Harper R, Land DG, Griffiths NM, Bate-Smith EC. 1968b. Odor qualities: A glossary of usage. *Brit J Psychol.* 59(3):231-252.
- Harper R, Bate-Smith EC, Land DG, Griffiths NM. 1968c. A glossary of odor stimuli and their qualities. *Perfum Essent Oil Rec.* 59:22-37.
- Hazzard FW. 1930. A descriptive account of odors. *J Exp Psychol.* 13(4):297-331.
- Henning H. 1916. *Der Geruch*. Leipzig, Germany: Barth.
- Heyninx A. 1919. *Essai d'Olfaction Physiologique*. Brussels: Larcier.
- Jaubert JN, Tapiero C, Doré JC. 1995. The field of odors: toward a universal language for odor relationships. *Perf Flav.* 20(3):1-16.
- Jellinek P. 1951. *Die Psychologischen Grundlagen der Parfümerie*. Heidelberg: A Hüthig Verlag.
- Jellinek JS. 1992. Perfume classification: A new approach. In: Van Toller S, Dodd GH, editors. *Fragrance: The Psychology and Biology of Perfume* London: Chapman & Hall. p. 229-242.
- Jeltema MA, Southwick EW. 1986. Evaluation and applications of odor profiling. *J Sens Stud.* 1(2):123-136.
- Jennings-White C. 1984. Human primary odors. *Perf Flav.* 9(6):46-58.
- Klein S. 1947. Primary odor element classification. *Am Perf Essent Oil Rev.* 50:453-454.
- Linnaeus C. 1756. *Odores medicamentorum*. In: *Amoenitates Academicae*, Vol. 3. Stockholm, Sweden: Lars Salvius. p. 183-201.
- Lovell JH. 1923. Classification of flower odors. *Am Bee J.* 63: 392-394.
- MacDonald MK. 1922. An experimental study of Henning's system of olfactory qualities. *Am J Psychol.* 33(4):535-553.
- Moncrieff RW. 1966. *Odor Preferences*. London: Leonard Hill. p. 219.
- Richardson A. 1999. Measurement of fragrance perception. In: Pybus DH, Sell CS, editors. *The Chemistry of Fragrances*. Cambridge, UK: The Royal Society of Chemistry. p. 145-157.
- Rimmel E. 1895. *The Base of Perfumes*. London. (French translation 1990, *Le Livre des Parfums*. Paris: Les éditions 1900).
- Ross S, Harriman AE. 1949. A preliminary study of the Crocker-Henderson odor-classification system. *Am J Psychol.* 62(3):399-404.
- Rowe D. 2000. More fizz for your buck: High-impact aroma chemicals. *Perf Flav.* 25(5):1-19.
- Schutz HG. 1964. A matching-standards method for characterizing odor qualities. *Ann NY Acad Sci.* 116:517-526.
- Sell CS. 2004. Scent through the looking glass. *Chem Biodivers.* 1(12):1899-1920.
- Thiboud M. 1991. Empirical classification of odors. In: Müller PM, Lamparsky D, editors. *Perfumes: Art, Science, and Technology*. New York: Elsevier. p. 253-286.
- von Haller A. 1763. *Classes odorum*. In: *Elementa Physiologiae* Vol. 5, book 14, section 2. Lausanne, Switzerland: Grasset. p. 162-168.
- Yoshida M. 1975. Psychometric classification of odors. *Chem Senses.* 1(4):443-464.

- Zarzo M. 2013. What is a fresh scent in perfumery? Perceptual freshness is correlated with substantivity. *Sensors*. 13(1):463-483.
- Zarzo M, Stanton DT. 2009. Understanding the underlying dimensions in perfumers' odor perception space as a basis for developing meaningful odor maps. *Atten Percept Psycho*. 71(2):225–247.
- Zwaardemaker H. 1925. *L'Odorat*. Paris: Doin.



**Table 1** Common categories of pleasant odors considered by different authors

Code	Odor category	References
1	Fragrant:	LI, BA, ZW, CR, HA
1.1	- Balsamic (vanilla-like)	RI, HE, BI, HA
1.2	- Floral (flowery)	LO, BF, KL, BI, AM, HA
2	Aromatic:	LI, LO, ZW, HA, JW
2.1	- Camphoraceous	RI, ZW, AM, HA, JW
2.2	- Spicy	RI, HE, ZW, HA, JW
2.3	- Aniseed	RI, ZW, JW
2.4	- Citrus	RI, ZW, BF, HA, JW
2.5	- Almond	RI, ZW, HA, JW
3	Ambrosial:	LI, ZW, KL
3.1	- Amber	RI
3.2	- Musky	RI, LO, AM, HA, JW
4	Alliaceus (garlic, onion)	LI, HE, LO, ZW, BF, HA, JW
5	Hircine (goat-like, caprylic)	LI, ZW, CR
6	Ethereal (etherish)	BA, HE, ZW, AM, HA, JW
7	Empyreumatic / burnt	HE, ZW, CR, BF, BI, HA, JW
8	Woody	RI, KL, BI, HA, JW
9	Fruity (non-citrus)	RI, LO, KL, BI, HA, JW
10	Herbaceous (herbal)	RI, KL, HA
11	Green	HA, JW
12	Menthollic (minty)	RI, BF, AM, HA, JW
13	Earthy, fungoid	KL, HA
14	Oily / fatty	HA, JW
15	Fishy	HA, JW
16	Sour, acid	CR, HA, JW
17	Pungent, sharp	AM, HA, JW

Codes 1-7: odor classification proposed by Zwaardemaker (1925)

References: AM (Amoore 1962), BA (Bain 1855), BF (Bienfang 1941), BI (Billot 1948), CR (Crocker and Henderson 1927), HA (Harper 1975), HE (Heyninx 1919), JW (Jennings-White 1984), KL (Klein 1947), LI (Linnaeus 1756), LO (Lovell 1923), RI (Rimmel 1895), and ZW (Zwaardemaker 1925).

## FIGURE LEGENDS

**Figure 1.** Odor Cube showing typical perfumery descriptors. Gray regions delimit the four basic categories proposed by Crocker and Henderson (1927): “fragrant” (upper left rectangle), “acid” (upper back square), “burnt” (upper front square), and “caprylic” (bottom front triangle). Descriptors located close to each other should in theory correspond to similar odors. Camphoraceous, alliaceous, and sulfidic odors are not properly represented in the cube; their link with the most closely related descriptors is indicated with arrows pointing away from the cube.

**Figure 2.** Projection of descriptors onto the base of the Odor Cube (Fig. 1) (filled circles, terms in boldface). Descriptors in italics (white circles) correspond to the Odor Effects Diagram (Jellinek 1951), and those in brackets correspond to a subsequent modification of this diagram (Calkin and Jellinek 1994). The loading plot showing the contributions in the formation of PC1 and PC2 for the descriptors in the B-H database (see Fig. 5 of Zarzo and Stanton 2009) is also depicted for comparison (triangles), and was rotated to achieve the best possible coincidence with Jellinek’s diagram.

**Figure 3.** (A) Relationship between the Odor Cube and different underlying dimensions in the descriptive space of smells. The brown colored area around the “earthy” corner is supposed to correspond to the most unpleasant odors, whilst the opposite applies to the magenta area. (B) Henning’s Odor Prism (1916). The reference material of each odor class (Gamble 1921) is indicated within brackets. White circles correspond to odor categories that can be matched in both representations.