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Qualitative Differences of Divalent Salts: Multidimensional Scaling and Cluster Analysis

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Abstract

Sensations from salts of iron, calcium, magnesium, and zinc with different anions were studied using a sorting task and multidimensional scaling (MDS). Ten divalent salts were adjusted in concentrations such that the mean intensity ratings were approximately equal. Stimuli were sorted on the basis of similarity to minimize any semantic influence and were examined with and without nasal occlusion to eliminate retronasal cues. Compounds representing the four primary tastes and astringency were also sorted. Similarity estimates were derived from sorting and were submitted to MDS. Divalent salts fell outside the area of the space defined by the four primary tastes. The nose-open condition showed that some of the divalent salts have unique metallic sensations along with astringency. The groupings obtained were corroborated using single-linkage cluster analysis. An iron group was most distinctive in metallic sensations; calcium and magnesium salts were primarily bitter; and zinc salts were characterized by astringency. When nasal cues were not available, the sensations from the divalent salts were mainly explained by bitterness and astringency. Results were consistent with a previous evaluation of divalent salts using descriptive analysis.

Key words: calcium, iron, magnesium, metallic taste, sensory characteristics, zinc

Introduction

The gustatory model of Henning (1916) is based on four primary tastes. The notion of four tastes had formed a theoretical basis for psychophysical and neurophysiological studies until a fifth taste quality, umami, was introduced. Other nontraditional oral sensations, such as astringency (Lee and Lawless, 1991; Breslin *et al.*, 1993; Green, 1993; Lawless *et al.*, 1996) and metallic (Schiffman, 2000; Lawless *et al.*, 2004, 2005; Lim and Lawless, 2005a,b; Yang and Lawless, 2005a,b), have been recently studied. Some oral sensory perceptions of divalent salts cannot be fully explained by a single taste or a mixture of four (or five) primary taste qualities. For example, a retronasally perceived metallic smell is a salient property of iron salts (Lawless *et al.*, 2004), and astringency is a major property of zinc salts (Keast, 2003). An increasing number of foods are fortified with minerals, and this practice often results in an unacceptable taste or flavor, for example, a metallic aftertaste. The success of nutritional fortification is thus linked to understanding the sensory properties of divalent salts.

The general consensus about the tastes of divalent salts is that they are complex (Lawless *et al.*, 2003). The cation is primarily responsible for the sensory characteristics of inorganic salts with modifying effects of the anion. In the case of some organic sweeteners such as cyclamates the anion can be the major contributor. Divalent salts differ in the predominance of metallic, bitter, and astringent sensations they evoke (Yang and Lawless, 2005a). Lawless *et al.* (2004) showed that retronasal smell is an important cue for perceiving metallic sensations from ferrous sulfate. Later, Lim and Lawless (2005b) reported that the sensations of ferrous salts are a complex of retronasal, gustatory, and possibly tactile cues and are changed as a function of concentration and anions. The oral sensory properties of divalent salts can be described by a combination of four basic tastes with the addition of metallic and astringent. Schiffman and Erickson (1971) classified calcium and magnesium chloride as bitter–salty. Lawless *et al.* (2003) characterized the taste of calcium and magnesium salts as primarily bitter taste, with additional sensations described as salty, metallic, astringent, sour, and sweet. Tordoff (1996) reported that 1 mM calcium chloride solution was rated as 35% bitter, 32% sour, 29% sweet, and 4% salty. He also commented that the taste of calcium varies with both the form and concentration of salt tested. The sensory mechanism of zinc seems to be different. Keast (2003) concluded that the zinc salts have very little taste (bitter, salty, savory, sour, and sweet), and astringency is the major oral sensation. Green and Hayes (2003) found magnesium chloride to have an irritative, burning component. In spite of this research on psychophysics of divalent salts, direct comparison of a wide array of salts with different qualities has been rare (Yang and Lawless, 2005a).

In most psychophysical studies, terms are generally preselected by the experimenter and not defined for subjects in order to avoid biasing them toward a particular response (O'Mahony and Thompson, 1977; Yang and Lawless, 2005a). O'Mahony and colleagues have shown that semantic issues are complicating in studies of taste quality and that the choice of words that are provided can influence descriptions and distort psychophysical results (O'Mahony and Thompson, 1977; Ishii and O'Mahony, 1987; Delwiche, 1996). Furthermore, taste qualities such as umami might be characterized as a case of concept learning rather than simple identity with a physiologically based taste-categorization scheme (O'Mahony and Ishii, 1987). Given these semantic complications, one approach is through descriptive analysis, which provides training and references to build a consensus vocabulary to profile sensory attributes (Meilgaard *et al.*, 1991). A trained descriptive panel evaluated developed a vocabulary and characterized the sensory qualities of 10 divalent salts (Yang and Lawless, 2005a). These data are valuable since they provide a comprehensive set of oral sensory attributes. Yet, semantic problems are not entirely solved, including panelist variation in ratings that persist even after training, some of which may be due to phenotypic variation (Lugaz *et al.*, 2002).

To avoid semantic problems, measuring the similarity of stimuli rather than using attribute ratings is an alternative approach. Multidimensional scaling (MDS) has been used in understanding the range of quality in the chemical senses (Schiffman and Erickson, 1971; Schiffman *et al.*, 1979, 1980; Kielhorn and Thorngate, 1999). MDS data can be collected as direct similarity ratings or by derived similarity scores from sorting (Lawless, 1989), and thus, it does not require ratings on specified attributes or subjective descriptions. MDS produces a spatial map, which reflects the relationships between stimuli in terms of their perceived characteristics.

Traditional procedures for collecting data for MDS can be time consuming and impractical since the number of paired comparisons for N stimuli is $[N(N-1)/2]$. However, a number of researchers have explored a simple sorting procedure as an alternative data collection and demonstrated that it is at least as effective as conventional procedures (Lawless, 1989; Lawless and Glatter, 1990; MacRae *et al.*, 1990, 1992; Lawless *et al.*, 1995; Stevens and O'Connell, 1996). In the sorting task, subjects examine the set of items and group them according to similarity (Lawless, 1989). Although the raw data have ordinal properties, they can be processed by MDS models to give quantitative information (Falahee and MacRae, 1997). A simple index of similarity can be derived from counting the number of times any given stimulus pair is sorted into the same category, summed across the panelists. The assumption is that similar items should be sorted together with high frequency, and dissimilar items should almost never belong to the same sorted group.

The primary purpose of this study was to clarify the perceived sensations from salts of the nutritionally important minerals, iron, calcium, magnesium, and zinc, and to gain a greater understanding of the contribution of the cation and anion to the sensory qualities. We assess whether these sensations are similar to the traditional sweet, sour, salty, bitter, and astringent oral qualities. The taste quality umami was not included since previous studies (Keast, 2003; Yang and Lawless, 2005a) showed that it was not a distinctive quality for the minerals mentioned above, although it was applicable to some extent for the zinc salts. Whether nasal occlusion would shift the perceptions of mineral salts in a similar manner to the reduction of metallic ratings of iron salts was also investigated. MDS analysis of sorting data was employed. The distances among the stimuli are representative of their perceptual interrelationships and reflect their similarity and/or dissimilarity. We expected classes of stimuli based on the predominant sensory character (e.g., bitter vs. metallic). Nasal closure was expected to affect the position of $FeSO_4$ due to its strong retronasal metallic aroma (Hettinger *et al.*, 1990).

Materials and methods

Subjects

The subjects were 19 students and employees at Cornell University, Ithaca, NY, aged 20–34 years (mean: 25, 14 females). All subjects were nonsmokers and free from anosmia by self-report. Panelists had prior sensory testing experience, although not in MDS. Subjects were asked not to eat or drink for at least 1 h prior to testing. A token incentive was paid at the end of testing. Panelists gave informed consent. The study was approved by the University Committee on Human Subjects.

Stimuli

The test stimuli (see Table 1) were 15 solutions in deionized water, including four basic taste stimuli, a mixture, one tactile stimulus, and nine divalent salts. Citric acid, sodium chloride, sucrose, quinine hydrochloride, and alum were used to represent sour, salty, sweet, bitter, and astringent sensations, respectively. A mixture of sodium chloride and quinine hydrochloride was also included to represent a salty and bitter taste that was expected to plot in an intermediate position between its components. A duplicate NaCl sample was included to test for reliability. Stimuli were prepared daily to prevent oxidation. Stimuli were presented as 20-ml samples in 60-ml odorless plastic cups (Solo 2 oz. Plastic Cups, Solo Cup Company, Urbana, IL) labeled with a three-digit random number at room temperature (approximately 21°C). Stimuli were sipped and expectorated.

Table 1 Formulae, sources, concentrations, and plot codes of the 15 stimuli

Stimulus	Formula	Source	Concentration (mM)	Plot code
Citric acid	$C_6H_8O_7{\cdot}H_2O$	Fisher Chemicals (Fairlawn, NJ)	3.0	CA
Sodium chloride	NaCl	J.T. Baker (Phillipsburg, NJ)	120	N
Sucrose	$C_{12}H_{22}O_{11}$	J.T. Baker (Phillipsburg, NJ)	400	S
Quinine hydrochloride	$C_{20}H_{24}N_2O_2{\cdot}HCl$	Sigma Chemical (St. Louis, MO)	0.08	Q
Mixture of sodium chloride and quinine hydrochloride			120 and 0.08	NQ
Aluminum ammonium sulfate	$AlNH_4\ (SO_4)_2{\cdot}12H_2O$	Sigma Chemical (St. Louis, MO)	2.0	AL
Calcium chloride	$CaCl_2{\cdot}2H_2O$	EM Science (Gibbstown, NJ)	25	CC
Calcium lactate	$CaC_6H_{10}O_6$	Fluka Chemika (Buchs, Switzerland)	150	CL
Ferrous chloride	$FeCl_2{\cdot}4H_2O$	J.T. Baker (Phillipsburg, NJ)	30	FC
Ferrous gluconate	$FeC_{12}H_{22}O_{14}{\cdot}2H_2O$	Alfa Aesar (Ward Hill, MA)	50	FG
Ferrous sulfate	$FeSO_4{\cdot}7H_2O$	J.T. Baker (Phillipsburg, NJ)	55	FS
Magnesium chloride	$MgCl_2{\cdot}6H_2O$	J.T. Baker (Phillipsburg, NJ)	30	MC
Magnesium sulfate	$MgSO_4{\cdot}7H_2O$	EM Science (Gibbstown, NJ)	150	MS
Zinc chloride	$ZnCl_2{\cdot}2H_2O$	J.T. Baker (Phillipsburg, NJ)	10	ZC
Zinc sulfate	$ZnSO_4{\cdot}7H_2O$	J.T. Baker (Phillipsburg, NJ)	20	ZS

Procedures

The experiment was divided into two parts: three sessions of intensity matching and four sessions of a sorting task. Each session lasted approximately 25–30 min. Testing sessions were conducted in individual booths under red light to eliminate any visual differences.

Intensity matching

To begin the session, subjects were told to rinse their mouths with deionized water and then to taste a stimulus for a few seconds and expectorate. They rated the overall intensity of the stimulus on an unstructured line scale (1000 pixels, about 18 cm on a computer screen) marked with "weak" and "strong" at each end. Scores were converted to a 0–10 basis in 10ths; thus, a rating at weak was transcribed as "0.0" and a rating at strong as "10.0." During a 1-min break in between stimuli, subjects were asked to rinse their mouths with deionized water. Concentrations which yielded geometric means between 4.6 and 5.6 were considered to be approximately equal in overall intensity. Data were collected using Compusense five (version 4.4.8, Compusense, Inc., Guelph, Ontario, Canada). The intensity matching also served as a familiarization process to illustrate the range of perceived qualities from the stimuli.

Sorting task

Each subject attended four testing sessions; two sessions with a nose clip and another two sessions without a nose clip, in counterbalanced order and occurring at least 1 day apart. As it was not feasible for the panelists to finish sorting in one session, the experiment was conducted over 2 consecutive days for each condition to minimize fatigue and cross-adaptation effects. Subjects were allowed to leave the testing when they felt fatigue and resumed their work the next day at the same time. Subjects were presented with a fresh tray of stimuli for each session. The test was conducted under red light to mask any color cues from the stimuli.

Each subject was given a tray with all 16 stimuli (including the duplicate NaCl) in random order. An instruction sheet, an illustrative example of a taste-sorting test, and a sheet for recoding responses were provided. Subjects tasted the stimuli in any order as many times as they wished and sorted them into groups of stimuli having similar taste qualities. As a memory aid, paper and pencil were provided for their personal notes. A minimum of two groups was required, but there was no other constraint on the number of groups they could make. When they had completed the sorting, participants recorded their responses by writing down the three-digit codes for each group of samples in separate columns and provided a few words to describe the differentiating attributes for that group of stimuli. They were encouraged to taste them again to check that they were satisfied with their final groupings. Panelists were allowed to taste and sort the samples at their own pace and were instructed to rinse between samples with deionized water. Unsalted crackers were also available for palate cleansing.

Analysis

The number of times each possible pair of stimuli was placed in the same group was summed across the 19 panelists to form a group index of similarity. This produced half-matrices submitted to SYSTAT 5.2 (Wilkinson, 1991) using the non-metric MDS option (Kruskal, 1964), a procedure similar to KYST. Two-dimensional (2-D) and three-dimensional (3-D) solutions were computed. Single-linkage cluster analysis was also performed on the data using Minitab (2003). Cluster analysis was used to help interpret the groupings in the MDS configurations by an objective method.

Results

Similarity spaces based on sorting data

Subjects formed 6–10 categories (mean: 7.6, SD: 1.17) for the nose-open condition and 5–10 categories (mean: 6.9, SD: 1.29) for the nose-closed condition. Stress values in the MDS configurations and R^2 values for the 2-D and 3-D configurations are shown in Table 2. A 3-D solution was chosen since the stress value was low, and the R^2 was improved from the 2-D to the 3-D configuration. The stress value for the nose-closed condition was higher, suggesting that the data were less clearly structured. Figures 1 and 2 show the MDS configurations for the nose-open and the nose-closed conditions, respectively. Dissimilarity is represented by distance: stimuli that are close together are perceptually similar.

In the nose-open condition, subjects put the NaCl duplicates in the same group, and therefore, they plotted at the same spot. Also the mixture of salty and bitter stimuli was plotted between NaCl and quinine (QHCl), as expected. The divalent salts fell outside the area of the space defined by the sweet (sucrose), sour (citric acid), salty (NaCl), and bitter (QHCl) standard. Each cation with different anions tended to group together. Ferrous salts ($FeCl_2$, $FeSO_4$, and Fe gluconate) were arranged closely together; magnesium salts fell between QHCl and ferrous salts; zinc salts were located close to alum, the astringent standard; and calcium salts were plotted near QHCl as well as alum.

The most distinctive difference between the two nose conditions occurred with the ferrous salts (comparing Figures 1 and 2). $FeSO_4$ moved from the edge of the spatial arrangement with the nose open toward the center, which is closer to QHCl, in the nose-closed condition. $FeCl_2$ also repositioned between citric acid and QHCl. Other stimuli were arranged similarly with the nose-open condition, although the overall configuration appeared less systematic.

Cluster analysis of MDS coordinates was performed to identify groupings. The hierarchical dendrograms are shown in Figures 3 and 4. Seven clusters were obtained for the nose-open condition and five clusters for the nose-closed condition. Sucrose, NaCl, and citric acid were separated into three clusters and were dissimilar from the divalent salts for both the conditions. In the nose-open configuration, there

Table 2 Stress and R^2 values for the 2-D and 3-D configurations

	2-D configuration		3-D configuration	
	Stress	R^2	Stress	R^2
Nose open	0.10	0.95	0.04	0.99
Nose closed	0.09	0.96	0.07	0.97

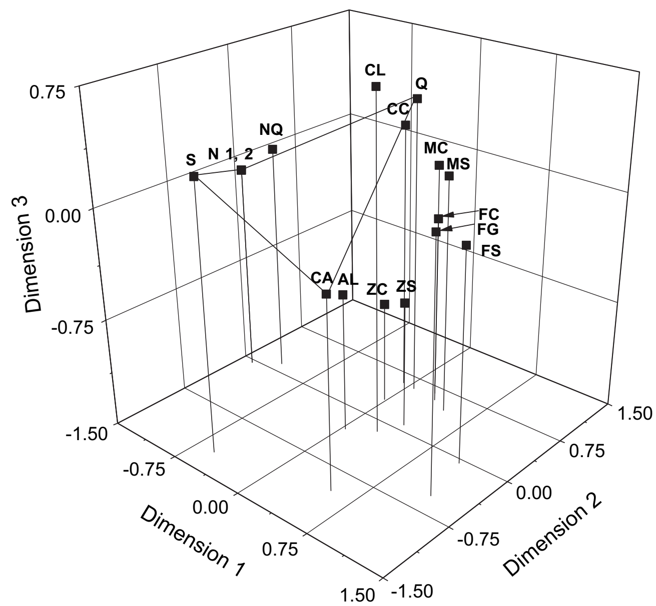

Figure 1 3-D Kruskal solution for the nose-open condition. Letters refer to stimuli as designated in Table 1.

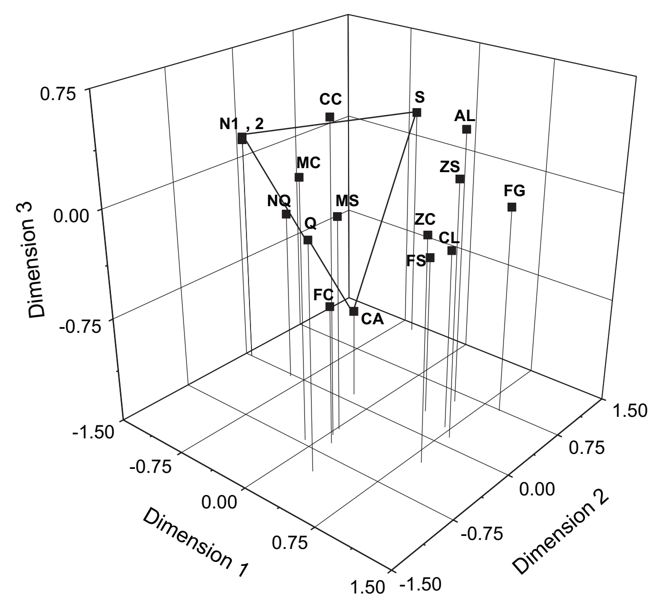

Figure 2 3-D Kruskal solution for the nose-closed condition. Letters refer to stimuli as designated in Table 1.

were four distinctive clusters among divalent salts: a bitter group (Quinine, $CaCl_2$, $MgCl_2$, $MgSO_4$, and $FeCl_2$), an astringent group (alum, $ZnCl_2$, and $ZnSO_4$), a metallic group (Fe gluconate and $FeSO_4$), and calcium lactate. In the nose-closed condition, the configuration was simpler. One cluster was the bitter group as above. A second cluster included the astringent stimuli plus the metallic (Fe) group and finally calcium lactate (by itself). One stimulus from the metallic group, ferrous gluconate, was on the side of the cluster closest to citric acid, possibly due to its sour contribution from the formation of gluconic acid (Yang and Lawless, 2005a).

Descriptions of stimuli

Verbal descriptions of sorted groups are shown in Table 3. While the labels for the common taste or tactile stimuli were quite similar among the subjects, those for the divalent salts were more variable. Subjects tended to describe the test stimuli with the labels of "bitter," "sour," "salty," or "astringent." Most of the other adjectives were common descriptions of metallic sensations (e.g., dirty coin taint, rusty iron, and rancid), tactile sensations (harsh, sharp, and pungent), and chemical (chemical like, mineral like, and poison like). The most idiosyncratic labels were caramel, burnt, or smoky describing ferrous gluconate. Some subjects commented that zinc salts are meaty or umami. There were several subjects that described a few of the test stimuli, especially $FeCl_2$, as neutral, bland, or "no flavor" when they wore the nose plugs. On the whole, nose-open and nose-closed conditions were similar, except for the metallic compounds. Metallic-related descriptors decreased in the nose-closed condition, consistent with the absence of a metallic retronasal smell (Hettinger *et al.*, 1990; Lawless *et al.*, 2004).

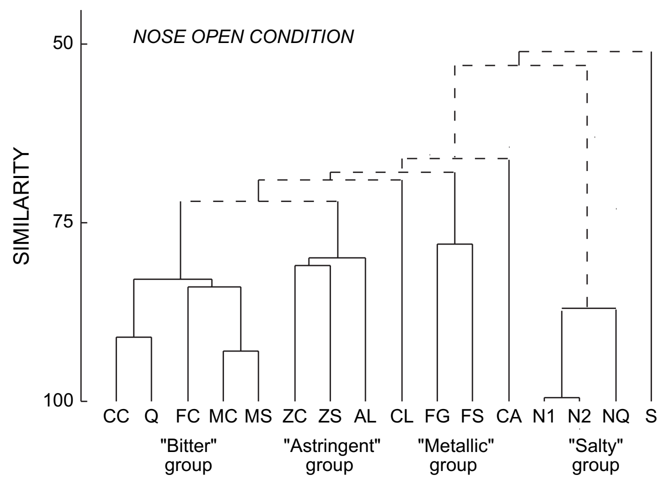

Figure 3 Dendrogram produced by hierarchical cluster analysis of the 3-D coordinates in the MDS solutions of Figure 1 using the single linkage.

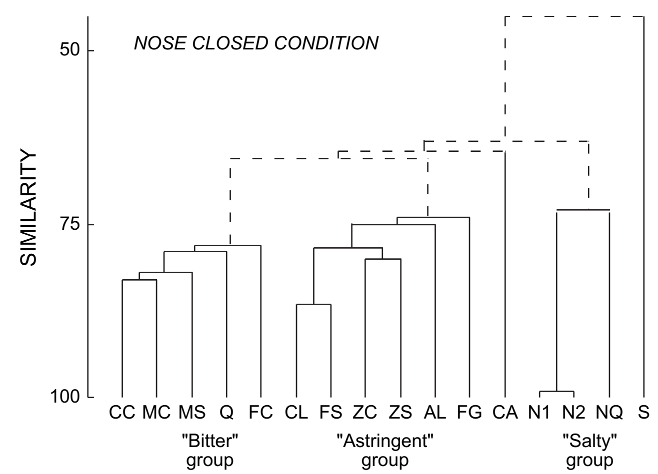

Figure 4 Dendrogram produced by hierarchical cluster analysis of the 3-D coordinates in the MDS solutions of Figure 2 using the single linkage.

Discussion

Sensations elicited by the 10 divalent salts were mapped using MDS for comparison to traditional sweet, sour, salty, bitter, and astringent stimuli both with and without retronasal cues. The primary question was whether some of the stimuli would fall outside of a gustatory model, the taste tetrahedron, which is bounded by four primary tastes at each corner (Henning, 1916). With the nose open, divalent salts were clearly located outside of the gustatory model. Divalent salts may be poorly characterized by a simple combination of four standard tastes as suggested by Schiffman and Erickson (1971). Yang and Lawless (2005a) conducted a descriptive analysis of a similar set of divalent salts. The visual configuration from principal component analysis in their Figure 6 was well matched with Figure 1 from this study (after rotation left by 90°). In that study, the iron group was characterized by metallic taste and metallic aftertaste; the zinc group was described as astringent, umami, and spicy; and magnesium and calcium were primarily bitter. The sensory characteristics of divalent salts appear to be a combination of retronasal, gustatory, and tactile (astringent and possibly irritative) sensations.

Some iron salts produce a retronasal metallic smell (Hettinger *et al.*, 1990; Lawless *et al.*, 2004). The iron group, especially iron sulfate and gluconate, were plotted away from the four primary tastes domain toward the right side of the first dimension (Figure 1). This distinctive group disappeared, and the iron salts repositioned depending upon their anion when the retronasal cue was not available. Thus, dimension 1 in the nose-open condition might be characterized by a metallic smell. However, in the nose-closed condition this dimension is less clear. Some salts, calcium lactate, ferrous sulfate, ferrous gluconate, zinc chloride, and zinc sulfate, were positioned at the right side of dimension 1 along with the astringent alum in the nose-closed condition. A good proportion of the descriptors used for those salts with nasal closure were metallic, spoiled, aftertaste, chemical like, medicine like, and harsh. Dimension 1 might still be related to metallic

Table 3 Common descriptor choices (number of subjects)

Stimulus	Nose open	Nose closed
Citric acid	17 sour, 4 astringent	16 sour, 7 astringent
Sodium chloride	19 salty	19 salty
Sucrose	19 sweet/sugary	19 sweet/sugary/syrupy
Quinine hydrochloride	17 bitter, 4 astringent	19 bitter, 3 astringent
Mixture: NaCl/QHCl	17 salty, 6 bitter	17 salty, 10 bitter
Alum	13 astringent/drying, 9 sour	13 astringent, 10 sour
Calcium chloride	13 bitter, 3 salty, 3 astringent	15 bitter, 3 sour, 3 bland/neutral
Calcium lactate	7 bitter, 6 sour, 5 astringent, 5 sweet	10 sour, 10 bitter, 6 astringent, 3 sweet,
Ferrous chloride	12 bitter, 10 astringent, 6 metallic	14 bitter, 6 astringent, 3 no flavor/bland,
Ferrous gluconate	12 metallic, 7 sour, 5 astringent, 4 sweet	9 sour, 6 astringent, 5 metallic, 4 sweet,
Ferrous sulfate	10 metallic related, 7 astringent, 4 bitter	8 astringent, 7 sour, 7 bitter
Magnesium chloride	13 bitter, 7 astringent/drying, 6 metallic	16 bitter, 5 astringent
Magnesium sulfate	12 bitter, 6 astringent	17 bitter, 5 astringent
Zinc chloride	14 astringent, 7 bitter	12 astringent, 7 bitter
Zinc sulfate	11 astringent, 7 bitter, 5 metallic	11 astringent, 6 bitter, 4 sour

Sour includes related terms such as acidic, tart. Astringent count includes drying. Metallic related includes iron, rusty. Lower frequency choices are omitted.

sensations, but in a broader sense, consistent with the suggestions (Lim and Lawless, 2005a; Yang and Lawless, 2005a) that perception of metallic sensations can subsume an array of perceptions including aroma, a taste quality, and mouth feel.

Astringency is a salient property of this stimulus set. Alum was plotted in the vicinity of citric acid in the normal tasting condition. Organic acids are often both astringent and sour (Lee and Lawless, 1991; Lawless *et al.*, 1996). Alum moved to the right side of dimension 2 when the nasal flow was unavailable, more distant from citric acid. Astringency was perhaps more prominent when the nose was closed, which is also suggested by the cluster analysis.

The properties of each salt are diverse, but there is some consistency within salts having the same cations (Yang and Lawless, 2005a). Iron salts evoked metallic (rusty iron, penny like, fishy, and rancid), astringent/drying, bitter (especially for the chloride), sour, and chemical-like sensations (Hettinger *et al.*, 1990; Lawless *et al.*, 2004; Lim and Lawless, 2005a,b; Yang and Lawless, 2005a,b). Zinc salts were mainly considered astringent as found by Keast (2003) with some other qualities such as burning/hot/sharp, bitter, salty, metallic, and umami. When monosodium glutamate (MSG) was shown as a reference in descriptive analysis to illustrate the umami concept, zinc salts were perceived to have this quality (Yang and Lawless, 2005a), although Keast (2003) found limited application of the "savory" descriptor. In retrospect, it would have been interesting to have included MSG and see it if plotted near to the zinc salts. Tastes of calcium and magnesium have long been believed as bitter–salty (Moncrieff, 1967; Schiffman and Erickson, 1971), and the result from cluster analysis as well as the position near to quinine in Figure 1 indicated a similarity to bitter stimuli.

Lawless *et al.* (2003) concluded that calcium and magnesium salts were primarily bitter, but with additional sensations described as salty, metallic, astringent, sour, and sweet.

Although each cation with different anions grouped together, the variations in the anion resulted in differences in the overall sensations of these salts especially with nasal closure. The most distinctive phenomenon regarding anion was that the divalent salts with chloride were located closer to the quinine compared to the same salts with other anions. $FeCl_2$ was near the other iron salts in Figure 1, although cluster analysis grouped $FeCl_2$ with bitter stimuli. Yang and Lawless (2005a) concluded that bitter tastes were pronounced for the calcium and magnesium salts and for ferrous chloride. Tordoff (1996) and Lawless *et al.* (2003) observed a decreased bitterness of lactate or other organic anions on calcium or/and magnesium salts (compared with chloride) and described this effect as anionic inhibition. They explained this phenomenon in two possible ways; the effect of large organic anions preventing calcium from acting on receptor sites (Nakamura and Kurihara, 1991) and the inability of larger anions to diffuse across paracellular junctions and into basolateral areas of taste receptor cells (Ye *et al.*, 1991, 1993; Delwiche *et al.*, 1999). The gluconate anion also has complicating characteristics and possibly a sour contribution. Previous findings (Lim and Lawless, 2005a;

Yang and Lawless, 2005b) showed that the ferrous gluconate salt evoked a larger percentage of sour responses than did the other salts, chloride, and sulfate. This phenomenon was explained by the formation of ferrous hydroxide and gluconic acid with a dissociable hydrogen ion when ferrous gluconate was dissolved. Iron gluconate also has a unique flavor quality. Several subjects described this salt as sweet, caramel, smoky, and burnt. Gluconate is the anion of gluconic acid, which is the carboxylic acid form of glucose. Therefore, these sensations could be caused by similar impurities to those derived from glucose during processing (i.e., volatile caramelization products producing various "sweet" smells). Because none of the other salts have this quality, ferrous gluconate is positioned slightly apart from the other salts. Since the metallic flavor was very strong, this quality might not be given much attention in the nose-open condition. On the other hand, when sensory differences between stimuli are more subtle, any cue that is discriminable may be emphasized.

A final issue in this research concerns the use of MDS via a sorting task for basic psychophysics. The blended stimulus was located between its component stimuli, and the replicates plotted in the same position in the space. These results confirm the reliability and reasonableness of the sorting procedure. Although there is no ready method for determining the intrinsic meaning of the dimensions plotted in these similarity spaces, the spatial maps seem interpretable combined with the results from cluster analysis and comparison to the descriptors that were selected. The results are also comparable to those obtained with descriptive analysis of a similar set of divalent salts. Figure 1 was visually well matched with a principal component analysis configuration from descriptive analysis (Yang and Lawless, 2005a). The sorting method is very simple and quickly performed by untrained subjects. A further advantage of this procedure is that it does not require any selection of attributes in advance (O'Mahony and Thompson, 1977; Falahee and MacRae, 1995). This is an important advantage when the stimuli are not familiar to the subjects and their vocabulary may be limited.

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