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Odor Thresholds

for Chemicals with Established Occupational Health Standards

3rd edition

*Provides important reference information for chemicals,
focusing on odor perception and other factors.*

Edited by
Sharon S. Murnane
Alex H. Lehocky, MS, CIH
Patrick D. Owens, CIH, CSP



HEALTHIER WORKPLACES | A HEALTHIER WORLD

Table of Contents

Preface v

About the Authors vii

Acknowledgments..... ix

Introduction..... xi

1. Anatomy and Physiology of Odor Perception..... 1

2. Odor Perception 3

 2.1 Dimensions of Odor.....3

 2.2 Properties of Olfactory Functioning5

 2.3 Variability of Olfactory Perception5

3. Role of Odor Perception in Occupational Settings 10

 3.1 Indoor Air Quality..... 10

 3.2 Respirator Use..... 10

 3.3 Workplace & Environmental Exposure Assessments..... 11

4. Odor Threshold Methodology..... 14

 4.1 Odor Measurement Standards and Methods..... 14

 4.2 Variability of Threshold Values 15

 4.3 Modeling 19

 4.4 Criteria for Review of Odor Measurement Technologies 21

5. The Literature Search and Review..... 23

6. Explanation of the Tables 25

References..... 26

Table 6.1. Odor Threshold Values 44

Table 6.2. Methods Summary of Reviewed Articles..... 91

Table 6.3. Reported Odor Thresholds from All Sources..... 118

Table 6.4. Odor Character List200

Table 6.5. Chemical Synonyms211

Table 6.6 Chemical CAS Number221

References for Table 6.2227

Preface

Estimates of odor threshold are still important to industrial hygiene, occupational safety, air pollution control and ventilation engineering. Since the original 1989 AIHA® publication on Odor Thresholds⁽¹⁾ and the 2nd edition⁽²⁾, there have been enough changes in testing methodology, occupational exposure limits and odor perception research to indicate a need for a revision.

An extensive literature review and critique occurred in the original publication. For the second edition, the literature examination consisted of methods review for those acquired articles.⁽²⁾ Numerous publications in odor research were published in the years since the original AIHA® book. Several of these references supporting the same information on odor variability were cited as the most current references in the second and third editions. The odor threshold values ranges were broad in some cases. So, caution in relying on odor alone as a warning of potentially hazardous exposures is strongly encouraged.

This third edition includes: some new odor threshold values, global exposure limits, expanded odor descriptors, description of quality threshold studies, information on estimating thresholds, summary of interindividual variability in threshold values, and modeling of thresholds based upon molecular structure. For those substances with many reported thresholds, the scattered values may give the impression that human thresholds vary widely. However, recent research shows the contrary. Using good objective methods and study design, thresholds were determined to vary much less than commonly believed.⁽³⁾

This publication is meant to provide the industrial hygiene practitioner with insight into the variables that affect the human perception to chemical odors in the occupational environment and guidance on good quality threshold data. The use of descriptive statistics, as in the original publication, was outside the scope and purpose of this 3rd edition, due in large part to the limitation of comparable data and multiple experimental methods used.

Sharon S. Murnane
Retired CIH & CSP

Alex H. Lehocky, MS, CIH
Director, Environmental Health & Safety
Kennesaw State University

Patrick D. Owens, CIH, CSP
Safety Engineer
Shell Oil Products US
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Introduction

This publication is intended to serve as a chemical odor threshold reference for use by industrial hygienists and other health and safety professionals.

There are several threshold value compilations available.⁽⁴⁻¹¹⁾ Some transform the original data for use while others record the range of threshold values. In the original AIHA® publication, critiquing the experimental odor threshold determinations reported in literature provided a basis for developing an estimate of odor threshold and represented the data available in odor threshold compilations at the time.⁽¹⁾

The third edition presents a range of odor threshold values for 311 odorant chemicals for which there are published occupational exposure limits. There were 182 chemicals in the original publication and 295 chemicals in the 2nd edition. The references used for occupational exposure levels are the OSHA Permissible Exposure Limits (PELS)⁽¹²⁾, ACGIH® Threshold Limit Values (TLVs®)⁽¹³⁾, NIOSH Recommended Exposure Levels,⁽¹⁴⁾ German MAK Commission⁽¹⁵⁾, OARS Workplace Environmental Exposure Levels™ (WEELs)⁽¹⁶⁾, and European Union Community Occupational Exposure Limits.⁽¹⁷⁾ The listing of odorous chemical thresholds in this publication is by no means a comprehensive compilation of all odorous chemicals or odor threshold data. The *Compilation of Odor Thresholds in Air and Water*, published by Gemert 2011, is a comprehensive source of peer reviewed research for 1921 chemicals with reported odor thresholds in air.⁽¹¹⁾ The Gemert document is the major basis for sources of odor threshold data reviewed in this publication. In addition, a thorough literature review was conducted that incorporated additional citations for thresholds, methods, variables, and human factors.

Industrial hygienists should understand the importance of odor science. IHs may be involved in decisions regarding what substance(s) to allow in the workplace. Besides referencing occupational exposure limits, knowing the odor thresholds for the choices available may prove extremely helpful in substance selection. Workers noticing odorants in the workplace may complain, or at least question, exposure limits and measured concentrations, which may prevent or minimize significant exposures and subsequent health effects. Thus, odor data can lead to closer scrutiny of substances to augment comparative analysis with Occupational Exposure Limits, if available.

Odor threshold research is an evolving science. As the technology of olfactometry and analytical measurement advances, threshold experiments are conducted and reported in the literature. Careful consideration of reported literature values is warranted due to differences in research techniques, the compounds studied, the study groups used, and various other factors explained later in this publication. Historically and even today many of the published odor threshold values can suffer due to the lack of control of important variables. Some detection thresholds, for example, were

determined for a particular chemical to have several orders of magnitude. Inadequate or lack of control of these variables, therefore, can lead to skepticism and little confidence among IH practitioners for using odor thresholds. Recent research shows the variability is due to lack of the following areas: odorant dilution, measuring the odorant's airborne concentration, delivery of blanks to control for false positive responses, delivering enough air so no overbreathing dilution occurs, and use of forced-choice responses. Lack of control over these variables generally leads to higher threshold values than reality. For example, if not enough odorant airflow is delivered to the person and overbreathing dilution occurs, the person would notice the odorant at lower concentrations than actually presented. Some researchers have found human odor thresholds highly reliable, reproducible, and with low variance if the important variables are controlled.⁽¹⁸⁾ To generalize, this research has suggested the most accurate estimate of a chemical's odor detection threshold is the lowest concentration reported using good methodology. If one uses the lowest value published, the study thus reporting this concentration should at least have measured the delivered concentration, used force-choice methods, provided sample blanks, and delivered the odorant such that the person could not dilute the sample.

A reported odor threshold is a concentration of odorant expected to be either detected or recognized by 50% of people with normal olfactory function. Usually, the threshold value isn't a concentration that is measured, but a statistical value estimated by the researcher. Good threshold studies include a large group of test subjects with the test concentrations spanning a wide enough range to account for normal human variability and low enough to include the most sensitive individual. Odor thresholds have been shown to be represented by lognormal distribution. Most studies do not specifically state the reported threshold is a geometric mean, but it is the unstated assumption. Well-designed studies require the subject to identify the odorant source among two or three choices. When the subject correctly chooses the odorant over the pure air at 100% of the trials, the detection probability is 1 (perfect detection). Likewise, when a subject fails to detect the odorant except by chance, the detection probability is zero. A psychometric function is developed where the odor threshold is the concentration of odorant detected by the evaluation panel at half-way between chance detection (i.e., detection probability = 0) and perfection detection (i.e., detection probability = 1).⁽¹⁹⁾ For each individual, threshold values should be determined from multiple repeated tests (i.e., typically three), with enough rest time between stimuli presentations to allow for recovery. Ideally, an odor threshold study should graph each test subject's geometric mean plotted versus concentration. This allows for an understanding of the average threshold and the variation between individual subjects. Older studies (i.e., 30–40 years ago) may have lacked the test methodology and statistical analysis to estimate the geometric mean. While this publication reports the range of the acquired odor threshold values, the reader is cautioned with regard to the reliance on the older studies unless the study has been reviewed for the correct statistical methodology.⁽²⁰⁾

Section 1 has information on the anatomy and physiology of odor perception. Section 2 presents material on odor perception and odor properties. Section 3 discusses the role of odor perception in occupational and environmental settings. In Section 4 a review of odor threshold methodology is given. Section 5 describes the literature search and review procedure conducted in the original publication. Section 6 presents the data tables of acquired odor threshold values and associated information.

1. Anatomy and Physiology of Odor Perception

Chemosensory perception is an important system for evaluating our environment. The sense of smell has been postulated to be one of the oldest senses.⁽²¹⁾ In human anatomy, olfaction (sense of smell) depends on the interaction between the odor stimulus and the olfactory epithelium. The structural design of the nose directs inspired air toward the olfactory epithelium located in the roof of the posterior nasal cavity. Perception of smell is based on the recognition and discrimination of the odorant molecules in the environment. In the olfactory system, thousands of genes encode olfactory receptors for this recognition and discrimination of odororous compounds.⁽²²⁾ Two olfactory organs are in the nasal cavity on either side of the nasal septum. Air is drawn into the nose, where it swirls around the nasal cavity. Such turbulent action causes airborne compounds to contact the olfactory organs. The compounds must diffuse into the mucus where they stimulate the olfactory receptors. Olfactory receptors contain neurons with cilia protruding from the surface. Chemicals interact with the receptors sending a response to the cerebral cortex in the brain.⁽²³⁾ Odor detection and perception occur because of olfactory receptor neurons located in the nasal epithelium. Receptor recognition of an odorant is overseen by the detection of the physico-chemical properties of the odor molecule.⁽²⁴⁾ When sensing odors, olfactory receptor (OR) proteins translate chemical information into neuronal signals that are decoded in the olfactory cortex and give a person an image of the odor.⁽²⁵⁾

A human has about 10–20 million olfactory receptors. Recent studies suggest that human olfactory sensitivities and neurobiology do compare well than those of other vertebrates like rodents and dogs.⁽²⁶⁾ While the human olfactory system is very sensitive, the activation of an olfactory receptor does not necessarily lead to sensory perception or awareness of the odorant. Inhibitions along the olfactory pathway can stop the sensations from reaching the olfactory cortex in the brain.

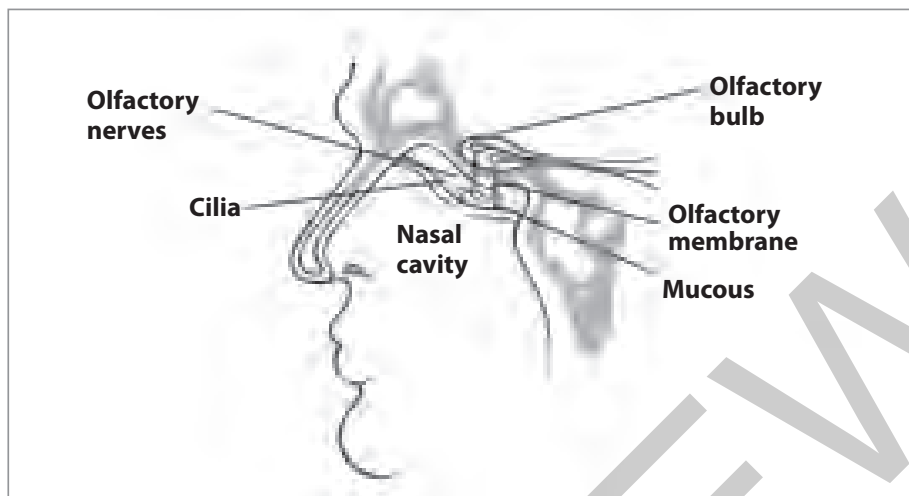


Figure 1.1. Anatomy of Smell.

<http://www.atsdr.cdc.gov/HAC/landfill/html/ch3.html>

Odor adaptation is the ability of the olfactory system to adjust its sensitivity at different stimulus intensities.⁽²⁷⁾ Odor adaptation occurs when a person becomes accustomed to an odor, so their threshold is altered. The odor detection threshold typically increases with adaptation. However, the odor recognition threshold can decrease after familiarity.⁽²⁸⁾ Adaptation will occur differently with each odorant. Odor fatigue occurs with prolonged exposure and when total adaptation has occurred.⁽²⁹⁾ Adaptation is often overlooked in olfactory testing. During testing, adaptation may cause a temporary decrease in smell function reflected in an increase in threshold value.⁽³⁰⁾

The earliest stage of olfaction is the sniff which is a reflex caused by chemicals and the simple transport means carrying odors to the olfactory receptors. Sniffing influences olfactory intensity, odor identity and quality perception. Neurological and psychiatric disorders that are accompanied by smell dysfunction might be related to impairments of sniffing. Natural sniffing provides optimal chemosensory perception. Sniffing prepares the olfactory receptor network for incoming chemosensory information.⁽³¹⁾ A sniff sends air into the olfactory epithelium where odorant molecules bind to olfactory receptors turning the chemical information into a neural signal. Sniffing influences quantity and quality of molecules perceived, impacts perception and drives neural activity patterns through the olfactory system.⁽²⁷⁾

2. Odor Perception

A brief review of the sensory properties of odor and some of the attributes of human olfactory response is presented to facilitate understanding of odor threshold values.

2.1 Dimensions of Odor

Odor is the feeling in the brain produced by the recognition of a chemical by an odorant receptor.⁽²¹⁾ Odor is the sensation created by stimulating the olfactory organs.⁽¹⁾

An odorant is any substance that can provoke an olfactory response. A chemical/molecule can be considered an odorant if it satisfies the following conditions⁽²¹⁾:

1. It must bind to a receptor.
2. The odorant receptor must convey the recognition to the brain.
3. The brain must recognize it as an interpretable signal.

The sensory perception of odorants has four major dimensions: **threshold, intensity, character, and hedonic tone (valence)**.⁽¹⁾

Odor threshold is the minimum gas-phase concentration of an odorant that generates a discerning response. Odor thresholds are substance specific and can vary over an extensive range.⁽³²⁾ Threshold values are relative. Several of the factors on which odor threshold values depend seem to be laboratory measurement factors and not intrinsic biological factors, such as⁽³⁰⁾:

- Stimulus dilution method
- Concentration step sizes
- Duration of the stimulus
- Molecule species
- Psychophysical task categories
- Time between stimulus presentations
- Number of test trials

Odor detection threshold, in general, is an estimate of the lowest concentration of odorant that 50% of the study panel will detect approximately 50% of the time. Detection thresholds do not require identification of the odor.^(30,33) The psychometric function is that odor threshold is the concentration detected by a panel at half-way between chance detection and perfect detection.⁽¹⁹⁾ The **odor recognition threshold** is the minimum concentration that is recognized by 50% of the evaluation panel.⁽³⁰⁾ Threshold values reported in the literature are statistical points typically representing the best estimate median value from a group of individual responses.

4. Odor Threshold Methodology

4.1 Odor Measurement Standards and Methods

Where odorant threshold values (i.e., detection, recognition or irritation) are given, the method used to obtain the value followed some type of standard should be noted. It is more likely, but not always the case, the older the published value, the less rigorous the methodology. There might have been one or more aspects (e.g., insufficient recovery time between challenges) of the test method that was not followed.

The current consensus standards for determining odor thresholds are:

- EN 13725–2003. Air Quality. Determination of Odor Concentration using Dynamic Olfactometry. This European Standard (EN) defines a method for the objective determination of the odour concentration of a gaseous sample using dynamic olfactometry with human assessors. The primary application is to provide a monitoring accuracy and results precision framework in olfactometry and has become the preferred method in Europe.^(32,187-190)
- ASTM E679-04. Standard Practice for Determination of Odor and Taste Thresholds by a Forced-Choice Ascending Concentration Series Method of Limits.⁽¹⁹⁾
- ASTM E544-10. Standard Practices for Referencing Suprathreshold Odor Intensity. These practices are designed to outline two preferred procedures for referencing the odor intensities of any odorous material in the suprathreshold region on the ASTM Odor Intensity Referencing Scale.⁽¹⁹¹⁾
- ISO 13301–2018. Sensory analysis – Methodology – General Guidance for Measure Odour, Flavor, and Taste Detection Thresholds by Three Alternative Forced-Choice Procedure.⁽¹⁹²⁾ The focus of ISO 13301:2018 is on data requirements and on computational procedures through general rules and precautions. It does not differentiate between detection and difference thresholds. ISO 13301 does not measure a recognition threshold and does not address the standardization of methods as discussed in EN 13725.

In the Forced-Choice Method, trained panel members receive odorous samples among clean samples. Test subjects are required to identify the presence of an odor. The detection threshold is the level at which a panelist can tell the difference between the diluted odorant and the clean sample. This method minimizes response biases and typically produce more reliable threshold values.⁽³⁰⁾ The researcher Nagata developed an accurate and simple method referred to as the Japanese Triangle odor bag method that includes forced-choice.⁽¹⁴⁶⁾

Some researchers refer to their methodology as olfactometry that is an effect-based measurement method to determine the human perception of an odorant.⁽³²⁾ An olfactometer is a dilution system in which the odor sample is presented to the assessment panel members.⁽³²⁾ The odorant is generated at a higher concentration and accurately

diluted before presentation to the test subject. The concentration always start low (i.e., most diluted) and gradually increases until detected 100% of the time by most test subjects. With olfactometry, the research operator controls the sample delivery while the test subject inhales through a sniffing port to detect the presence of odor.⁽¹⁸⁾ Most olfactometers are used in a laboratory setting.

Performing a detailed odor threshold study using a standard takes time, resources and equipment. There are other rapid techniques (e.g., squeeze bottles⁽¹⁹³⁾, essence cards⁽¹⁹⁴⁾, Sniffin sticks⁽¹⁹⁵⁻¹⁹⁹⁾) for evaluating human response to odorants. In general, these methods have been used for comparing odor thresholds between two or more study populations. For accurate comparisons, the researcher must ensure consistent objective testing criteria between the study groups. An electronic nose is currently in use by food, beverage and perfume industries. Although the electronic nose may appear to be less sensitive than olfactometry, there is a potential for use in odor evaluation.⁽²⁰⁰⁾

There have been efforts to do field evaluations of odors, usually, for evaluating public exposure environmental sources. A field evaluation of two methods of determining odor concentrations from mink farms found the portable dynamic olfactometer, Nasal Ranger, and Scentroid SM110 compared favorably to approximations using the psychophysical Weber-Fechner equation.⁽²⁰¹⁾ Some of these techniques use dilution to threshold methodology whereby the test subject is presented with a descending odorant concentration. How many dilutions (i.e., decreasing concentrations) required before the test subject no longer detects the odorant is the measurement. The more accurate methods use dilutions with carbon-filtered air.

4.2 Variability of Threshold Values

Historically, researchers did not actually measure the exposure concentrations but estimated them from chemical/physical properties such as vapor pressure. There are numerous possible errors introduced by such methodology. Research using vapor generation devices and mass-flow controlled systems reduces the chances of methodology errors and thus provides for more accurate predictions of thresholds.

Many factors can affect the results of olfactometry measurements. The relevant parameters are⁽³²⁾:

1. Device (e.g., olfactometer): accuracy, dilution steps, flow rates, etc.
2. Reference odorant(s)
3. Panel members
4. Assessment area: air quality, temperature, quietness

Accurately determining a chemical's odor detection threshold requires controlling and measuring many variables, such as:

- A panelist's performance in detecting odors is relative to the true concentration delivered. Therefore, it is important to accurately measure odorant concentration in any detection threshold evaluation.⁽²⁰²⁾
- Olfactory fatigue is the temporary, normal inability to distinguish an odorant after a prolonged exposure to that airborne compound. Olfactory fatigue can occur in a short period of time depending on the odorant.^(141,142)
- Untrained participants had higher detection thresholds than trained/experienced panelists. The untrained participants gradually lowered their detection thresholds through the exposure trials over time.⁽⁵⁵⁾
- Olfactometers should deliver a high enough flow rate to overcome subjects' ability to overbreathe the odorant and dilute it.⁽²⁰³⁾
- The type of solvent used for dilution of the odorant is important, so the diluent does not interfere with the odor detection results.⁽²⁰⁴⁾
- Regarding the presentation method, a study compared detection thresholds to PEA using both the staircase paradigm and a constant stimuli method of presenting dilutions in random succession. This study found no significant difference in PEA detection thresholds using these methods, and the constant stimuli method saved some time.⁽²⁰⁵⁾
- The persons conducting the odor measurements can influence the results and conclusions from the same environmental situation.⁽²⁰⁶⁾
- Two field olfactometers were evaluated in an exposure chamber and found to produce detection thresholds like measured concentrations.⁽²⁰⁷⁾
- One study examined eye and throat recognition/irritation thresholds to glutaraldehyde over varying exposure durations and found it affected thresholds slightly.⁽²⁰⁸⁾
- A comparison between detection thresholds for PEA and butanol using alternative test methods found phenyl ethyl alcohol (PEA) could be used as an alternative to butanol. Also, the wide-step method with fewer challenge dilutions compared favorably to the traditional narrow-step, many dilutions, presentation method.⁽²⁰⁹⁾ In contrast, another study found significant differences in odor detection thresholds between PEA and butanol.⁽¹⁰⁷⁾

Figure 4.2.1 illustrates the odor data variability one might expect from a well-designed study with normal subjects. This demonstrates that even a large percentage of people may have approximately a ten-fold difference in thresholds. The vertical axis label %t correct detection doesn't imply the test subject was incorrect when failing to detect the odorant. In this particular test, the test subjects had to choose among three nose cones which one was delivering the odorant. The figure illustrates that odor thresholds are best described by a lognormal distribution. Industrial hygienists should note the variability that can exist even in a controlled study and consider how much more variability might be found between workers in a typical workplace.⁽²¹⁰⁾

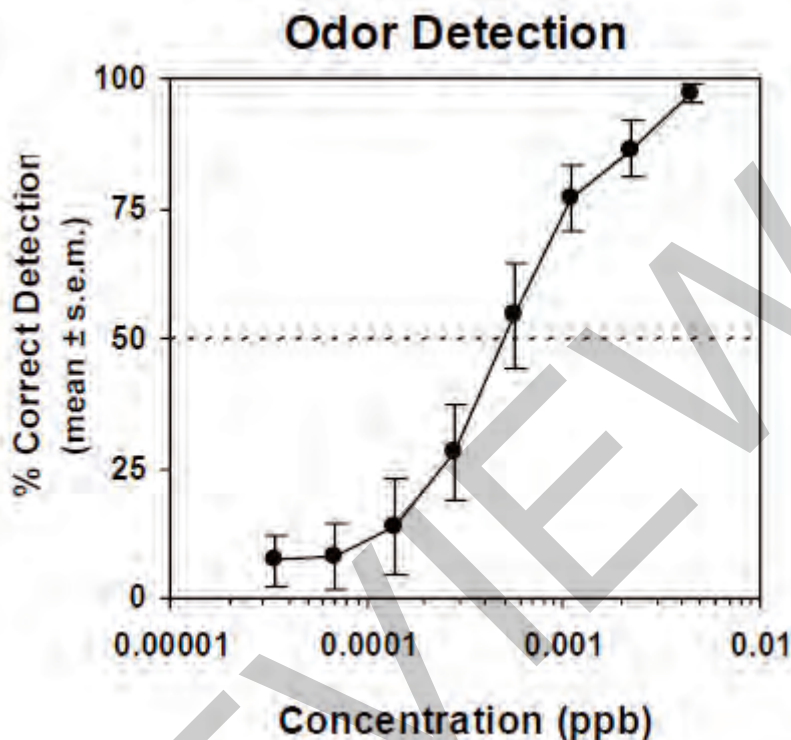


Figure 4.2.1 – Odor data variability.

Figure 4.2.2 illustrates four test subjects (i.e., S1, S2, S3, S4) and their percentage of times choosing the correct delivery cone with the odorant using eight different odorant concentrations.⁽¹⁸⁾ There is some percentage of random correct sample choices in this forced-choice method. Each test concentration is repeated several times. Each dot on the curve is a calculated average of all of an individual's repeated tests of that concentration. In a well-designed study, each of the individual results are combined to derive the psychometric function for the study population. Interindividual variation occurs as the result of several personal factors (e.g., age, gender, etc.). These human variability factors have been discussed in Section 2.3.1.

Ethyl Butyrate: Individual Subjects

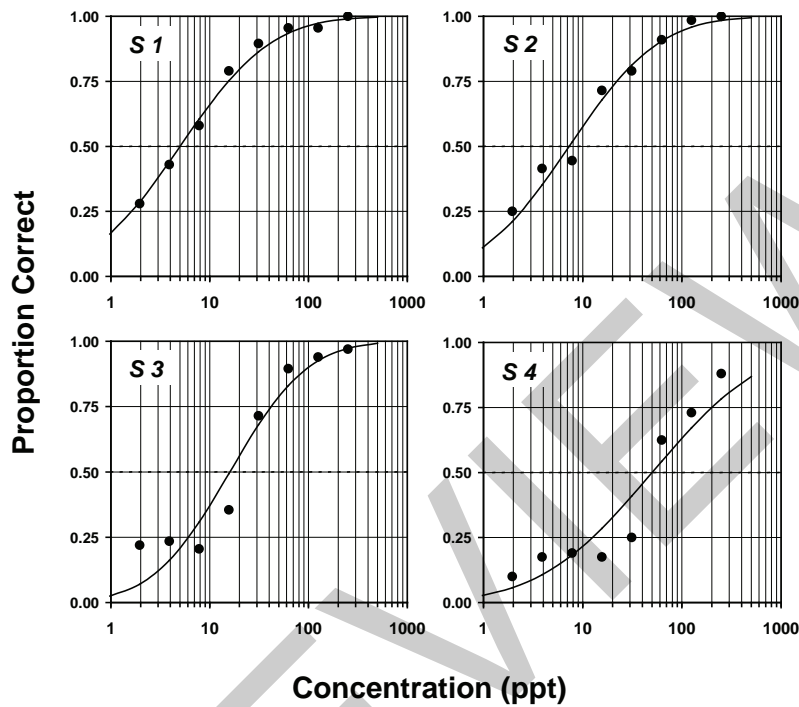


Figure 4.2.2 – Four test subjects and their percentage of times choosing the correct delivery cone.

The variation between an individual's threshold changes depends upon the odorant to some degree. Deficiencies in study method tend to raise the threshold due to issues like subject overbreathing (dilution), odorant degradation, odorant adsorption on equipment, not enough time for subjects to recover, and other issues. If the researchers are consistent in their test methods, threshold variability among the research findings show comparative consistency to each other.⁽³⁾

A Vapor Delivery Device ^{8(18,211)} in a laboratory setting is shown in Figure 4.2.3. This system design was based on decades of olfaction testing and continual improvements in methodologies to achieve the most accurate threshold data. The glass nose cones are designed to deliver the test concentration at a high enough flowrate to avoid velocity impact and prevent subject overbreathing leading to dilution of the test concentration and overestimating of the true threshold concentration.



Figure 4.2.3 – Vapor Delivery Device 8 (Courtesy of Dr. William S. Cain, Chemosensory Perception Lab, La Jolla, CA.)

4.3 Modeling

Modeling techniques for determining odor detection and eye and nasal irritation thresholds are under development and refinement. Correlating well with odor thresholds, algorithm equations were developed to help estimate odor thresholds in the absence of actual odor measurements.^(147,210,212,213) Hundreds of measured odor detection thresholds, verified by leading researchers in this field, were compared to the model estimates. Correlation coefficients above 0.7, sometimes as high as 0.9, were determined. These models have included various classes of volatile organic compounds. One of these models, based upon gas to condensed phases, has these independent variables: solute excess molar refractivity, solute dipolarity/polarizability, hydrogen bond acidity and basicity, and gas to hexadecane partition coefficient. These independent variables have been obtained from experimental data. Furthermore, researchers have determined the value of this constant for several different classes of VOC spanning hundreds of compounds. Overall, the efforts to develop models to estimate detection thresholds have been impressive. Recent research continues to add to the models' validity.

4.3.1 Quantitative Structure-Activity Relationship (QSAR)

Quantitative structure-activity relationship has the capacity to describe and eventually predict, olfactory and chemesthetic detectability functions in humans.⁽²⁰⁾ QSAR studies on the connection between molecular structure and odor threshold were modeled on numerous families of odorant molecules.^(106,153-157,176,180-182,210,214,215) However, the systematic interpretation of the models is challenging to perform because of the olfactory system complexity.⁽²¹⁵⁾

In 1996, Abraham published a method for estimating nasal irritation based upon a molecule's quantitative structure-activity relationship (QSAR). This article described a solvation equation to estimate sensory potency based upon a molecule's electron pairs, dipolarity/polarizability, hydrogen bond acidity and basicity, and hydrophobicity. The authors' speculated that the parameters described not only the ability of a compound to reach the nasal tissues, but also, the VOC solubility in the aqueous-lipid phase of the mucosal epithelium.⁽²¹⁶⁾

Nielsen, in 2007, published a review of occupational exposure limits set for eye or nasal irritation and the toxicology data used to derive the OEL. This article also discussed many aspects of the risk assessment process in establishing an OEL including the agent's odor threshold, irritation threshold, No Observed Adverse Effect Level (NOAEL), uncertainty factors (UF), Reference Dose (RD50), and QSAR estimation methods.⁽⁴⁹⁾

Jakubowski *et al.*, compared the irritant-based ACGIH® TLVs® against estimated nasal irritation values. Jakubowski calculated the nasal pungency threshold for 71 volatile organic compounds for which there were ACGIH® TLVs® based on upper respiratory tract and eye irritation. Jakubowski states that occupational exposure limits for nonre-active volatile organic compounds could be predicted using QSAR equations.⁽²¹⁷⁾

4.3.2 Abraham Algorithm

In one of the most comprehensive examinations of QSAR, Abraham *et al.*, focused upon estimating nasal detection thresholds. Odor thresholds obtained from Nagata using the triangular bag method were used. The Nagata dataset of measured odor thresholds encompassed a wide range of types of compounds as well as homologous sets of compounds. Abraham developed an equation to estimate odor detection and irritation thresholds based upon data from 353 compounds.⁽²¹²⁾ This equation can be used to estimate odor detection thresholds from a chemical's molecular properties.

$$\text{Log} \frac{1}{\text{ODT}} = -1.434 + 1.077E + 0.990S + 1.088A + 1.490B + 1.373V + 3.777M + 1.820AL \\ + 1.453AC + 1.205UE - 2.168C1 + 1.554C1AL + 2.478C1AC + 1.933C2AL \\ + 1.013C2AC - 0.812HS \quad (4.1)$$

N = 353, R² = 0.701, SD = 0.912, F = 52.6, PRESS = 327.096, Q² = 0.651, PSD = 0.985

The variables are:

E = solute excess molar refractivity

S = VOC dipolarity-polarizability

A = effective hydrogen bond acidity

B = effective hydrogen bond basicity

V = the McGowan volume

M = mercaptans (enter a 1 in the equation if an RSH fragment is present, otherwise enter 0)

AL = aldehydes when measured by Nagata

AC = acids when measured by Nagata

UE = unsaturated esters when measured by Nagata

C1 = any compound when measured by Cometto-Muniz or Cain in the 1990s

C1AL = above C1 aldehyde compound

C1AC = above C1 carboxylic acid compound

C2AL = any aldehyde reported by Cometto-Muniz 2008 to 2010

C2AC = any carboxylic acid reported by Cometto-Muniz 2008 to 2010

HS = any compound when measured by Hellman and Small 1974

In 2013, Cain *et al.*, examined the odor detection prediction data and worked on expanding the type of compounds accounted for by the Abraham equation. The Vapor Delivery Device (VDD8) was used for stable nasal irritation results. This study adds evidence that the odor detection threshold prediction QSAR may have applications for more types of compounds than previously thought.⁽²¹³⁾

4.4 Criteria for Review of Odor Threshold Measurement Technologies

In the original publication, odor threshold measurement methods were evaluated in terms of their conformity to the following criteria.⁽¹⁾

The Panel. The panel size minimum of six per group is recommended. Panelist selection should be based on odor sensitivity to the chemical odorants in question. Panel odor sensitivity (panel calibration) should be measured over time to monitor individual discrepancies and to maintain panel consistency. Typically, subjects are expected to be told they are participating in an odor detection study (i.e., they are focused on odor detection only). However, Whisman, et al., compared distracted from focused subjects and found the former to have, on average, approximately 27 times higher odor detection thresholds.⁽⁹⁹⁾

Presentation Apparatus. Vapor modality is in the form of a gas-air mixture or vapor over an aqueous solution and is determined by the test purpose and in turn determines the presentation method. Diluent should be consistent with the chemical compounds tested and should not influence odor perception. Presentation mode should minimize additional dilution (ambient) air intake. Analytic measurement should accurately measure the concentration of odorant as it reaches the panelist.

Calibration flow rate and face velocity are important system calibrations. Flow rate of odorant should be of enough volume to stimulate fully the olfactory receptors. The face velocity at which the odorant is flowed at the panelist should be maintained at a flow barely perceptible by the panelist.

Presentation Method. Either detection or recognition threshold types are appropriate. Concentration presentation is important because olfactory adaptation occurs rapidly. Presenting concentrations in ascending order (from weaker to stronger) or allowing for long periods between exposures are common methods to control for adaptation. Trials should be repeated for reliability. The forced-choice procedure minimizes anticipation effects for thresholds by eliminating false positive responses. Concentration steps of odorants should be presented successively at concentration intervals no more than three times the preceding one.

5. The Literature Search and Review

In the 1989 edition of this publication, odor threshold values and references were reviewed as shown in Table 5.1.

Table 5.1 – Code Nomenclature from the 1989 Edition

Code	Description
A	Accepted value based on critique
B	Rejected value based on critique
C	Rejected source based on review: <ul style="list-style-type: none"> • Secondary Source Code — Secondary sources identified as papers in which an odor threshold value, noticeable odor or detectable odor is mentioned, but either is not determined experimentally or is not referenced in the paper. • Incidental Reference — Incidental reference is different than secondary source in that experimental work was conducted but not with odor thresholds • Passive Exposure — Workplace — A study conducted in the work environment to determine worker exposure levels to a variety of substances and differing concentration levels. • Passive Exposure — Experiment — Test chamber experiments designed to determine the permissible limits of worker exposure to various substances.
D	Omitted Sources: <ul style="list-style-type: none"> • Unpublished Data • Personal Communication • Anonymous References • Omitted References per Gemert 1982 • Pre-1900 References • References with compounds that do not have TLVs
E	Sources not Reviewed — Foreign language articles Sources not Acquired — Old, foreign periodicals or theses

As in the 1989 publication, the second edition established the use of the Gemert compendium, and it updates as the major reference source. The reader should keep in mind two considerations. First, the compilation of odor threshold values truly is a formidable task encompassing both an interdisciplinary and world-wide search. Second, although the Gemert compendium does not attain perfection as a source, it is by far the best compendium of threshold values published to date. Gemert has collected data, from a wide variety of countries; extracted thresholds from a wide variety of disciplines (e.g., industrial hygiene, psychology, sensory evaluation, food technology, clinical medicine, air pollution control, engineering, chemistry); and encompassed a century of research.

For the second edition, the literature examination consisted of a method's review for those articles published after 1989 that could be acquired. References were not critiqued as in the original publication because the authors chose to report all the data available and suggest the use of the lowest value when needed. The object of this

edition was to provide more education on odor thresholds through explanation of the variability in obtaining thresholds and emerging technology in odor measurements.

For the third edition, the literature examination consisted of a methods review for those articles published after 2012 that could be acquired. References were not critiqued as in the original publication because the authors chose to report all the data available and suggest the use of the lowest value when needed. The object of this edition was to provide education on quality odor measurement methods and mathematical estimation of odor thresholds. Industrial Hygienists should use their professional judgment and use the odor information presented appropriately.

6. Explanation of the Tables

Data tables begin after the references used in the text portion. A range of odor threshold values and occupational exposure limits are in Table 6.1. Table 6.2 contains the methods summary information from the acquired articles that were reviewed for this edition. Table 6.3 is the published odor threshold values for the 311 chemicals with occupational exposure values. Table 6.4 allows the user to find chemicals by a description of the odor character. Table 6.5 allows the user to find a chemical name by a synonym. Table 6.6 allows the user to find a chemical by Chemical Abstract Number (CAS).

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Table 6.1 – Odor Threshold Values

The table contains the following information:

- Chemical Name, CAS Number, Chemical Formula, Chemical Molecular Weight
- Range of Referenced Odor Values
- Odor Character Description(s)
- OSHA Permissible Exposure Limit (PEL)
- ACGIH® Threshold Limit Value (TLV)®
- NIOSH Recommended Exposure Limit (REL)
- DFG MAK Value
- OARS WEEL™ Value
- EU Community Occupational Exposure Limit (OEL)

Abbreviations/Definitions used in the table:

- BEI® – Biological Exposure Indices
- C – Ceiling level that shall not be exceeded during any part of a working day
- DSEN – May cause dermal sensitization
- IFV – Measured as inhalable fraction and vapor
- H – Danger of percutaneous absorption
- RSEN – May cause respiratory sensitization
- Sa – Danger of sensitization of the airways
- Sah – Danger of sensitization of airways and the skin
- SEN - Sensitization
- Sh – Danger of sensitization of the skin
- Skin – Potential exposure by the cutaneous route
- STEL – Short Term Exposure Limit
- TWA – Time - weighted Average
- (W) – Worker exposure by all routes should fully be minimized

Table 6.1 – Odor Threshold Values

#	Compound Name CAS Number Formula Molecular Weight	Range of Odor Values (ppm)	Odor Character	OSHA PEL (ppm)	ACGIH TLV® (ppm)	NIOSH REL (ppm)	DFG MAK (ppm)	OARS WEEL® (ppm)	EU OEL (ppm)
1	Acetaldehyde 75-07-0 CH_3CHO 44.05	0.0015 – 1,000	ethereal, fresh, fruity, green, minty, musty, pungent, suffocating, sweet	TWA = 200	C = 25	—	TWA/STEL = 50	—	—
2	Acetic Acid 64-19-7 CH_3COOH 60.05	0.0004 – 204	acetic, acidic, pungent, sharp, sour, vinegar	TWA = 10	TWA = 10 STEL = 15	TWA = 10 STEL = 15	TWA = 10 STEL = 20	—	TWA = 10 STEL = 20
3	Acetic Anhydride 108-24-7 $(\text{CH}_3\text{CO})_2\text{O}$ 102.09	0.12 – 0.36	acid, sharp, sour, vinegar	TWA = 5	TWA = 1 C = 3	C = 5	TWA = 0.1 STEL = 0.2	—	—
4	Acetone 67-64-1 $(\text{CH}_3)_2\text{CO}$ 58.08	0.40 – 11,745	apple, chemical, etherous, fruity, minty, pear, sweet	TWA = 1,000	TWA = 250 STEL = 500 BEI	TWA = 250	TWA = 500 STEL = 1,000 H	—	TWA = 500
5	Acetonitrile 75-05-8 CH_3CN 41.05	13 – 1,161	aromatic, etherish	TWA = 40	TWA = 20 Skin	TWA = 20	TWA = 10 STEL = 20 H	—	TWA = 40 Skin
6	Acetophenone 98-86-2 $\text{C}_6\text{H}_5\text{O}$ 120.15	0.00024 – 0.59	acacia, almond, glue, hawthorn, mimosa, musty, oranges, pungent, sweet, river water	—	TWA = 10	—	—	TWA = 10	—
7	Acetylene 74-86-2 $\text{HC}\equiv\text{CH}$ 26.02	226 – 2,584	garlic, gassy	—	—	C = 2,500	—	—	—

Table 6.1 – Odor Threshold Values, cont.

#	Compound Name CAS Number Formula Molecular Weight	Range of Odor Values (ppm)	Odor Character	OSHA PEL (ppm)	ACGIH TLV® (ppm)	NIOSH REL (ppm)	DFG MAK (ppm)	OARS WEEL® (ppm)	EU OEL (ppm)
8	Acrolein 107-02-8 $CH_2=CHCHO$ 56.06	0.0027 – 1.8	almond, cherry, disagreeable, pungent	TWA = 0.1	C = 0.1 Skin	TWA = 0.1 STEL = 0.3	—	—	TWA = 0.02 STEL = 0.05
9	Acrylic Acid 79-10-7 $CH_2=CHCOOH$ 72.06	0.092 – 1.0	acid, plastic, randid, sweet	—	TWA = 2 Skin	TWA = 2 Skin	TWA/STEL = 10	—	TWA = 10 C = 20
10	Acrylonitrile 107-13-1 $CH_2=CHCN$ 53.06	1.6 – 22	garlic, onion	TWA = 2 C = 10 Skin 1910.1045	TWA = 2 Skin	TWA = 1 C = 10 Skin	H, Sh	—	—
11	Allyl Alcohol 107-18-6 $CH_2=CHCH_2OH$ 58.08	0.51 – 35	mustard, pungent	TWA = 2 Skin	TWA = 0.5 Skin	TWA = 2 STEL = 4 Skin	H	—	TWA = 2 STEL = 5 Skin
12	Allyl Chloride 107-05-1 $CH_2=CHCH_2Cl$ 76.53	0.48 – 5.9	pungent	TWA = 1	TWA = 1 STEL = 2 Skin	TWA = 1 STEL = 2	H	—	—
13	Allyl Isothiocyanate 57-06-7 $CH_2=CHCH_2NCS$ 99.15	0.0091 – 1.97	irritating, mustard, pungent, strong	—	—	—	—	STEL = 1 Skin, DSEN	—
14	Ammonia 7664-41-7 NH_3 17.03	0.043 – 60.3	ammoniacal, irritating, pungent	TWA = 50	TWA = 25 STEL = 35	TWA = 25 STEL = 35	TWA = 20 STEL = 40	—	TWA = 20 STEL = 50

Notes to Table 6.2

1. A project note about an experimental paper presenting threshold values.
2. Abstract with insufficient information.
3. Adaptation effects were avoided with a 45-min interval between concentrations.
4. Although a random presentation was used in this study, adaptation effects were avoided by presenting stimuli with 30-minute intervals between concentrations.
5. Approximate thresholds determined, and no threshold methodology is given.
6. Article focused upon validating olfactometer(s).
7. Article investigated whether subjects detected CO₂ in the nose or the mouth first.
8. Article investigates the odor detection, discrimination and chemesthetic properties.
9. Article investigating odor threshold differences between males, females, osmics and anosmics.
10. Article contains good descriptions for the compounds found in orange peel vapor.
11. Article investigating the compounds and their organoleptic intensity scales.
12. Article on good odor measurement methods/studies and the vapor delivery device 8 (VDD8).
13. Article refers to a minimal perceptible concentration based on an intensity scale.
14. Article refers to a previously published article for the details of the odor testing. Results are for brief, 2-minute duration, exposures only.
15. Ascending/descending patterns with consideration of other factors of the experimental design.
16. Concentration series are presented with insufficient time for de-adaptation of the olfactory receptors.
17. Concentration series not given, however the 1-hr waiting period used would eliminate adaptation effects.
18. Different subjects were tested at different concentrations to eliminate adaptation effects.
19. Evaluation of the repeatability of odor threshold data; determining the precision of odor threshold identification methods. Air-dilution olfactometer had good precision (4.2%).
20. German article. A tenfold concentration step size was used.
21. Flow rate difficult to determine.
22. Investigation of how the detection threshold might change when compounds are presented in mixtures.
23. Investigation of the properties affecting odor thresholds in hydroalcoholic solutions (like wine).

24. Investigation to identify and quantify the odorants from apples.
25. The MP is the minimum perceptible concentration of the most sensitive subject.
26. Number of subjects was insufficient to represent the range of olfactory sensitivity.
27. Only one concentration per day was tested to avoid adaptation effects.
28. Only the detection threshold for the Controls (without Alzheimer's disease) were quoted.
29. Panelists completed four scaling tasks in 30 min, with 10-sec waiting period between sniffs.
30. Participant count is the lowest number of subjects per compound.
31. Random presentation order to determine recognition threshold.
32. Results displayed on small graph in log ppb units; conversion errors may have resulted during conversion.
33. Russian article minimal perceptible value was determined from English summary.
34. Russian article was categorized based on translation of key words and review of tables presenting minimum perceptible values.
35. Study focus was testing olfactory fatigue between exposed and non-exposed workers.
36. Study investigated the odor threshold differences between smokers and non-smokers.
37. Study of the odor and chemesthesis (pungency and eye irritation).
38. Study of the odorant extracts of Lavage using GC-O.
39. Study on possible odorants for inert gas and investigated differences in age, sex, and smoking.
40. Study to compare the odor detection thresholds for smokers and nonsmokers.
41. Study to determine the odor recognition thresholds of several organics.
42. Study to identify the odor detection thresholds of common food odorants.
43. Study to identify the odor thresholds of chemicals in drinking water.
44. The study presents air values based on transformed data from water values and a descending series without adequate de-adaptation time.
45. Variable presentation was used with intervals between sniffs to reduce adaptation effects.
46. Threshold was calculated from the intensity slope at the intercept.
47. Thresholds were conducted as training for a field program. Threshold measurement recorded to document panel calibration.
48. Up-down technique used is less likely to cause olfactory fatigue than a descending or random pattern.
49. U.S. EPA Report on odor detection of methyl tert-butyl ether in water based upon on previously published data.
50. Investigation of the relationship between odor detection thresholds and age.

Table 6.3 – Reported Odor Thresholds from All Sources

Published odor threshold values for the 311 chemicals with occupational exposure values.

The table provides the following information:

- Chemical name in alphabetical order
- Source (Last name of first author) and publication date
- Type of odor threshold values reported as either detection (d) or recognition (r)
- Threshold values in both mg/m³ and ppm from the Gemert compendium and found articles published after 2012.

Note 1: Conversion of units from mg/m³ to ppm was based on the molecular weight of the compound and the known volume of a perfect gas or vapor at standard temperature and pressure (STP).

Note 2: The range of odor values can span several orders of magnitude. This edition reports all historic values that could be acquired and does not label any particular outlier values. If the user desires to calculate a geometric mean, appropriate evaluation of any outlier measurement should be made.

Table 6.3 – Odor Threshold Values (BOLD equals lowest value reported.)

#	Chemical Name	Source	Type of Threshold	Odor Thresholds	
				mg/m ³	ppm
1	Acetaldehyde	Zwaardemaker 1914	d	0.7	0.39
		Backman 1917	r	0.062 – 0.075	0.034 – 0.042
		Katz & Talbert 1930		0.12	0.067
		Balavoine 1943		10	6
		Pliška & Janiček 1965		1,800	1,000
		Gofmekler 1967, 1968	d	0.012	0.0067
		Leonardos et al. 1969	r	0.38	0.21
		Hartung et al. 1971		0.005	0.0028
		Takhirov 1974		0.49	0.27
		Teranishi et al. 1974		0.041	0.023
		Anon 1980	d	0.0027	0.0015
		Anon 1980	r	0.027	0.015
		Nauš 1982	d	1	0.555
		Nauš 1982	r	10	6
		Nagy 1991	d	0.09	0.05

Table 6.3 – Odor Threshold Values, cont. (BOLD equals lowest value reported.)

#	Chemical Name	Source	Type of Threshold	Odor Thresholds	
				mg/m ³	ppm
1	Acetaldehyde	Nagata 2003	d	0.0027	0.0015
		Yan et al. 2017		0.0390	0.0216
2	Acetic Acid	Passy 1893b, 1893c	d	5 – 10	2.04 – 4.1
		Grijns 1906		49 – 76	20 – 31
		Backman 1917	r	4.8 – 5.0	1.95 – 2.04
		Grijns 1919		2	0.81
		Mitsumoto 1926	r	0.074 – 0.57	0.030 – 0.23
		Hesse 1926	r	0.6	0.24
		Henning 1927	d	3.6	1.5
		Morimura 1934	r	1.82 – 1.91	0.74 – 0.78
		Jung 1936	d	0.025	0.01
		Jung 1936	r	0.05	0.02
		Balavoine 1943, 1948		300 – 500	122 – 204
		Stone 1963c	d	3.9	1.6
		Stone & Bosley 1965	d	4.2	1.7
		Endo et al. 1967		6.5	2.65
		Takhirov 1969, 1974		0.6	0.24
		Leonardos et al. 1969	r	2.5	1
		Homans et al. 1978		0.37	0.15
		Nauš 1982	d	0.5	0.20
		Nauš 1982	r	25	10
		Punter 1983	d	0.09	0.037
		Homans 1984		0.93	0.38
		Walker et al. 1990		5	2.04
		Nagy 1991	d	0.37	0.15
		Blank & Schieberle 1993		0.03 – 0.09	0.012 – 0.037
		Walker et al. 1996		0.25 – 2.5	0.1 – 1.0
		Cometto-Muñiz et al. 1998a	d	0.025	0.01
		Cometto-Muñiz 1999	d	0.025	0.01

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Odor Thresholds for Chemicals with Established Occupational Health Standards, 3rd edition

Edited by Sharon S. Murnane, Alex H. Lehocky, MS, CIH
and Patrick D. Owens, CIH, CSP

This review provides important reference information for chemicals with occupational exposure values, focusing on the anatomy and physiology of odor, odor perception, odor character, and a literature review of odor threshold methodology. Tables present information on the detection and recognition of odor thresholds, the experimental odor threshold determinations reported by each investigator and different ways to locate specific chemical information.

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