THE HANDBOOK OF CHEMICAL SUBSTITUTES

A Handbook of Substitutes and Alternatives for Chemicals and Other Commercial Products Including a Plan for Making a Proper Choice

by

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CHEMICAL PUBLISHING CO., INC.
New York, N.Y.

The Handbook of Chemical Substitutes

ISBN: 978-0-8206-0084-0 Paperback

Chemical Publishing Company:
www.chemical-publishing.com
www.chemicalpublishing.net

First Edition:

© **Chemical Publishing Company, Inc.** - New York 1985

Second Impression:

Chemical Publishing Company, Inc. - 2011

Printed in the United States of America

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Preface

Historically, this book was started about 40 years ago. At that time, the cosmetic, drug and flavor industries were seeking substitutes for glycerin and ethyl alcohol—for economic reasons and to avoid the red tape connected with the buying, storage, use, and selling of alcohol and alcoholic products. Fair substitutes were developed for both of these products, but when the price of glycerin was stabilized at a reasonable figure, these substitutes were almost completely forgotten.

Over a period of years, this writer has developed substitutes or alternatives for numerous products in diverse industrial fields. Thus, a file of such materials has been built up. To this has been added the suggestions of others and references from scientific and technical journals and texts.

This book cannot be regarded as complete or encyclopediac. The subject matter is in a state of flux and is growing and changing continuously. It should be useful to many as a starting point. It should not be expected to give the final answer to a highly specialized need. It is the task of the specialist or expert to glean from it what may be applicable and to interpret, interpolate, or "imagineer" a solution to his specific problem.

Condensation, rather than elaboration, has been the precept in assembling this information, in order to expedite the publication of this book. It is the concentrated essence of many years of experience of many chemists, engineers, and other technical workers.

This writer will greatly appreciate learning of any errors, omissions, or additions that might be made from those who use this book.

H. BENNETT

NOTICE

Introduction

Whether they be called substitutes, surrogates, replacements, or alternatives, such materials have been used from time immemorial. Sometimes they have been used to reduce costs; sometimes to replace unobtainable materials; and sometimes to produce better or different properties.

Selecting the proper substitute is no easy task. Since no material has all the same properties as the material which it will replace, it cannot be expected that the replacement will yield a finished product possessing exactly the same characteristics as the original. A replacement, therefore, that will produce a finished product which will perform almost the same function as the original, without too great a difference, is ordinarily considered satisfactory. For example, glycerin, in an antifreeze, has been satisfactorily replaced by ethylene glycol even though the two products differ in certain chemical and physical properties.

A substitute material, excluding price and availability, must be considered from many angles before it can qualify as a good substitute. Since it cannot have *all* the same physical and chemical properties as the original material, a compromise must be made. Thus, corn syrup may be suitable as a glycerin replacement in a suspending medium, where its viscosity is primarily desired, as in certain toothpastes. It is not of importance that corn syrup does not lower the freezing point of water or that it is not as hygroscopic as glycerin. Where, however, the last two factors or others are important, the use of corn syrup in place of glycerin, is not advisable.

Even when a suitable substitute is found, it may be necessary to modify the original formula by using a smaller or larger amount of the substitute and often, to add one or more other ingredients to balance it. Thus, because corn syrup is more viscous and less hygroscopic than glycerin, it may be necessary to reduce its viscosity by the addition of water and increase its hygroscopicity by means of a compatible hygroscopic salt. Introduction of these two additional ingredients may require considerable testing and aging to avoid subsequent undesirable effects.

Because of the uncertainty of the continued availability of any substitute material, it is advisable to try out a number of materials on each problem, so as to have a substitute ready for the substitute used. It means additional work, but is a worthwhile insurance for continuance in business.

Sometimes it may be desirable to change the composition of a formulation radically or entirely because a suitable substitution cannot be made. For example, flavoring extracts depend on the use of pure alcohol as the solvent for the flavoring ingredients. Since there is no good substitute for alcohol (in food products) available, a formuation without alcohol is indicated (e.g., lemon oil) made with an edible gum (gum tragacanth) and water. Of course, the finished product does not look like the original lemon extract, but it can replace it in most of its uses.

Price should not be too great a deterrent in selecting a substitute. Sometimes a substitute will alter a product so as to make it more useful, desirable and salable. An example of this is the use of monoglycollin in place of glycerin. Although the former is more than twice as expensive as the latter, its much greater solvency for certain dyes makes it far more economical to use than the cheaper material which it will replace. In electrolytic condenser manufacture, mannitol, at about three times the cost of glycerin, is replacing the latter because it gives a much more desirable product.

In getting outside assistance in finding a substitute, it is important to disclose a problem in its entirety. Reputable manufacturers and consultants hold all communications in strict confidence. Therefore, give them the complete formulation, method of manufacture, packaging, and a sample of the finished product. Also inform them how and where the finished product is to be used. Only with such complete information can an intelligent recommendation be made.

Substitute Requirements

Every chemical is unique in its chemical and physical properties. Therefore no chemical can replace another equally in all its characteristics. The following list which should be scrutinized gives most of the factors which must be considered in searching for a suitable substitute or alternative. Only those properties which are absolutely essential should be demanded; otherwise the search for a substitute will be greatly hampered, if not made futile.

Adhesion
Adsorption and Absorption
Availability
Bacterial Content
Boiling Point
Caking or Agglomeration
Carcinogenicity
Color
Compatability (Interaction)
Corrosiveness
Cryoscopic Properties
Density and Specific Gravity
Dispersing Properties
Drying Qualities
Edibility
Effect of Aging
Effect of Microwaves
Effect of Soundwaves
Effect of Ultrasonics
Effect on Animals and Plants
Effect on Bodily Functions (Other than Poisoning)
Effect on Skin, Hair, or Fingernails
Effects of Pressure
Elasticity
Electrical Properties
Emulsifiability
Explosiveness
Feel or "Hand"
Flexibility
Form
Freezing Point (Melting Point)
Gelling or Thixotropic Tendencies
Grade or Purity
Handling
Hardness
Heating Power
Homogeneity
Hygroscopicity or Efflorescence
Impurities
Inflammability
Interaction with Other Materials and Containers
Legal Restrictions
Length
Lighting Power (Candle Power)
Odor
Optical Properties
Patent Infringement
Plasticity and Ductility
Plasticizing or Flexibilizing Properties
pH
Polymerization

Radioactivity
Resistance to Oxidation
Resistance to Shock
Resistance to Ultraviolet
Resistance to Vibration
Slipperiness or Friction
Solubility
Solvency
Sound Conductivity
Stability
Static Properties
Stickiness
Sublimation
Surface Tension
Taste
Tenacity or Cohesion
Thermal Changes
Thermal Conductivity
Toxicity
Uniform Replacement
Vapor Pressure
Viscosity

AVAILABILITY

Unavailability is not a new phenomenon. Shortages or unavailability of certain materials have existed at certain times in various parts of the world—grain in Egypt during Biblical times; rice in China in modern times; oils and fats in Germany during the first World War; quinine, rubber, and other monopolistically controlled commodities because of restrictions in production and sale prior to World War II; silk, quinine, rubber, coconut oil, and many other raw materials due to crop failure, export or import prohibition, restrictions by producers or governments, unavailability because of rebellion or war.

Availability—the ability to get a material when and where it is wanted is of paramount importance. No matter how good a substitute may be, it is useless if not available. Therefore, the first step is to make sure that the substitutes to be examined are in plentiful supply, that they be preferably of domestic and not foreign origin, that the known suppliers will be able to take care of quantity requirements as needed.

With conditions being as they are today, it is seldom possible to plan ahead as far as raw materials are concerned. What is available today may soon become unavailable. However, since all consumers are subject to this same uncertainty, everyone is on an equal footing. That is why secondary substitutes must be decided on—in the event that the best substitute cannot be obtained.

HOMOGENEITY

Homogeneity implies uniform composition so that every part of a substance or mixture is of identical composition and appearance. Some products change in homogeneity because of differences in specific gravity, solubility, or for other reasons and produce a nonuniform condition. They must either be stabilized against such change or must be mixed or warmed to produce homogeneity before use. If the material is such that it cannot be brought back to its original state of uniformity (e.g., a decomposed glue), then it should not be used.

UNIFORM REPLACEMENT

Uniform replacement refers to the ability to obtain the same grade of product each time that it is ordered. Slight variations when unavoidable, may be compensated for, by technical control. Large or certain types of variations may make a product unusable. Thus, traces of copper are undesirable in materials used in rubber compounding. Consequently a material, which is the same in all respects, as previous deliveries, would be ruled out if contaminated with copper or its compounds. A material containing 0.1% of iron might be suitable for another purpose, but if the iron content increased to 0.5%, it may no longer be usable.

GRADE OR PURITY

The following grades of chemicals may be available:

C.P.
Commercial
Technical
Special
Natural
Synthetic
U.S.P.
Ultrapure
B.P.
Unofficial
N.F.
N.N.R.

C.P. stands for chemically pure. Each container usually bears a label of analysis, indicating the amounts of impurities present. This grade is usually the purest grade of chemical available. It is generally more expensive than the other grades but it is not specified except when high purity is required.

Commercial is the most common grade of chemical sold. Any chemical which does not bear a grade designation can be considered of commercial grade.

Technical is the ordinary commercial grade or some slight variation from it. This grade should not be used for food, drug, or cosmetic purposes without investigation.

Special refers to a particular grade made for a particular consumer or industry. It is different, in degree, from all other grades—either more or less pure. Its form and packaging may also be different.

Natural refers to a crude or refined product of vegetable, mineral, or animal origin; e.g., crude or resublimed iodine or camphor.

Synthetic refers to a chemical which is built up from a number of different chemicals by a chemical reaction process, e.g., synthetic menthol. A synthetic chemical usually contains fewer impurities than the corresponding natural product.

U.S.P. refers to the United States Pharmacopoeia, an official compendium giving the requirement for purity for many drugs and chemicals. A drug or chemical marked U.S.P. indicates that it meets all the specifications of the U.S. Pharmacopoeia.

Ultrapure refers to a most highly pure product.

B.P. refers to the British Pharmacopoeia, an official British compendium giving the requirements for purity for many drugs and chemicals. A drug or chemical marked B.P. indicates that it meets all the specifications of the British Pharmacopoeia.

Unofficial indicates that the drug and chemical has not been tested by the proper authorities and that it is not yet officially recognized in the pharmacopoeia.

N.F. shows that the product is listed in the National Formulary and is recognized by the American Pharmaceutical Association.

N.N.R. shows that the product is listed in New and Non-Official Remedies and is recognized by the American Medical Association.

FORM

Materials occur or are produced as gases, liquids, or solids. These are always the same under the same conditions of temperature and pressure. Gases and liquids usually do not exhibit any variation in appearance, handling, or use under similar conditions. Solids, however, do differ and may cause trouble. If they are crystals, the crystals may be large or small. A substitute may have a different crystalline form or shape (needle-like, cubic, etc.) which if used dry, may be undesirable because of appearance or bulking properties. Powders, likewise, consist of particles which may vary in size. Such variations not only affect appearance but also density, flow, agglomerating or "caking" tendencies, suspension, deposition, friction, and other properties.

OPTICAL PROPERTIES

Color (Shade, Intensity)
Clarity
Fluorescence
Phosphorescence
Iridescence (Pearliness)
Refractive Index
Reflectance (Dully, Shiny)

Color is of importance not only for appearance but also where staining, dyeing, or pigmentation occurs. The color of a material may vary with the size of the particles, larger particles being darker. Thus, crystalline copper sulfate is blue while the finely powdered material is a very light blue. Certain materials lose or change their color on being dissolved, dehydrated, or on interaction with another ingredient.

Clarity refers to clearness and freedom from haze or turbidity. Most commercial products are clear. Sometimes they develop a haze, turbidity, deposit, or a sediment, especially in metal containers. Others lose clarity even in glass containers because of polymerization (e.g., formaldehyde).

Fluorescence is the instantaneous re-emission of light from a substance of a greater wavelength than that of light originally absorbed. Common examples are seen in a solution of fluorescein in water and in certain types of mineral oils.

Phosphorescence is the re-emission of light, after a time lag, of a longer wavelength than that absorbed. This phenomenon is typified by the glowing of yellow phosphorus in the dark.

Iridescence is the rainbow-like play of colors as of pearls and soap bubbles.

Refractive Index is the relationship between the speed of light in a vacuum and its speed in a substance. The refractive index of a substance determines the degree of bending or distortion of an object viewed through the substance. Thus, it is of importance in adhesives for cementing optical glass, transparent plastics, etc.

Reflectance refers to the fraction of light which is reflected when light falls on any surface. Thus, a rough surface reflects very little whereas a smooth surface reflects more light. The former appears dull and the latter, shiny.

ODOR

Pleasant
Unpleasant
Strong
Faint
Temporary
Permanent

Odor is the effect on the sense of smell produced by particles emanating from a substance. In many products such as food, cosmetics, and household articles, odor is an important factor. Where an undesirable odor cannot be eliminated, it may often be "covered up" by a stronger, more desirable odor.

No odor is equally pleasing to all. Certain types of pleasant odors are bland, refreshing, or stimulating and are not objectionable in certain products. Unpleasant odors may be sickening, irritating, or depressing. An odor may be strong or faint. Faint, unpleasant odors are more tolerable than strong, unpleasant odors and may be masked more easily.

Very volatile odors may only be temporary and may disappear quickly on aging, storage, or use. Permanent odors must be recognized as an ever-present factor.

In blending various materials there may be a diminution of odor caused by the dilution or change in character or strength of the substance. These changes may result from decomposition or interaction with another ingredient.

TASTE

Sweet
Sour
Bitter
Salty
Spicy
Oily
Fruity
Neutral or Tasteless
Pleasant
Unpleasant
Strong
Permanent

Taste is a factor in those products that enter the mouth. Such products are foods, beverages, medicines, dentifrices, and certain cosmetics for the lips.

Pleasant tastes may be sweet (as in sweet chocolate); sour (as in lemon drops); bitter (as in hops, used in beer-making); spicy (as in ginger); salty (as in brine); oily (as in olive oil); neutral or tasteless (as in water); fruity (as in berries).

Just as with odors, strength and permanence are of importance and must be given due regard. An undesirable taste may often be "covered up" by a stronger or more desirable taste. Certain tastes which are unpleasant when too strong, are more pleasant when diluted, e.g., saccharine.

pH

pH is the logarithm of the reciprocal of the hydrogen ion concentration in gram molecules per liter or, more simply, a measure of acidity or alkalinity of a water solution of a substance. Pure water, which is neutral, has a pH of 7. Any pH above 7 is considered alkaline and below 7 is considered acid.

Thus, the pH of a solution of a material is indicative as to whether it is alkaline or acid and sometimes is a measure of its strength. This is a clue to how it will affect materials with which it is mixed or with which it may come into contact. Further details of the influence of acidity and alkalinity are given in the section on *Interaction With Other Materials.*

DENSITY AND SPECIFIC GRAVITY

Density is the weight per unit volume; e.g., pounds per cubic foot. Specific gravity is the relation between the weight of a given substance compared with the weight of an equal volume of water at the same temperature and pressure.

The density or specific gravity of a product varies with its purity, porosity, size of its particles, and the process by which it was made.

Density or specific gravity are critical factors where bulking, value, suspension, low cost, etc. are important.

Thus, calcium carbonate will vary in density or specific gravity depending on whether it is in the form of natural limestone, marble, or chalk, or a chemically precipitated product.

VISCOSITY

Viscosity is the resistance of a fluid to shear, agitation, or flow. More commonly it refers to rate of flow of a specific liquid as compared to water or any other commonly used liquid.

In some cases, viscosity is of importance because the greater the viscosity of a liquid the lower the rate of flow, spreading, penetration, wetting, etc., and the better its suspending power. A lower viscosity of course reverses these properties. A viscous liquid is harder to mix, fill, pour, and apply than a less viscous liquid.

Viscosity may be increased or lowered by suitable additions and treatments. Thus, the viscosity of mineral oil can be increased by heating it with some aluminum stearate; the viscosity of an alkaline casein dispersion can be reduced by means of urea. Other specific methods for altering viscosity are known and these should be used when a substitute is suitable in all other respects.

GELLING OR THIXOTROPIC TENDENCIES

Gelling is the formation of a gel or jelly-like substance; e.g., glue or agar with water. The thixotropic state refers to a gel which liquefies on shaking or stirring and which regels on standing; e.g., iron hydroxide or certain clay suspensions in water.

Gelling may be desired in certain cases as in hectograph (duplicating) compositions, whereas in the case of a paint, gelling, which would prevent brushing or spraying, is undesirable.

Gelling may be due to the colloidal properties of a single substance in a liquid (as with gelatin and water) or may result from the interaction of one or more substances (as with sodium silicate and dilute hydrochloric acid).

Gelling may be temporary, as in the case of a cold gelatin and water jelly, which becomes liquid on warming; or it may be more or less permanent as in the case of rubber cement (rubber swollen in a hydrocarbon solvent).

Gels may be thinned or prevented from forming by the addition of suitable agents. Thus, fish glue in water is prevented from gelling by the addition of acetic acid.

FREEZING POINT (MELTING POINT)

The freezing point is the temperature at which a liquid solidifies or begins to form crystals under normal conditions. Liquids containing impurities or added substances have different freezing points than the pure liquids. Therefore, the freezing point of a liquid is a measure of its purity. Similarly, if the freezing point of a substance is too high or too low, it may be altered by suitable additions.

The melting point is that temperature at which a solid changes to a liquid under normal conditions. The melting and freezing point of any substance is usually the same.

Some substances (mixtures), e.g., hydrogenated coconut oil, do not have a definite melting point but melt over a specific temperature range. Other substances soften or become plastic at certain temperatures; e.g., pitch, cellulose acetate, etc. Still others do not melt but sublime when heated sufficiently.

VAPOR PRESSURE

Vapor pressure is the pressure of any vapor above its liquid or solid form at the temperature at which equilibrium is established.

The greater the vapor pressure of a substance, the greater is its tendency to evaporate and disappear when exposed. High vapor pressure is desired in products which are expected to evaporate or dry quickly, as in cleaning fluids and lacquer thinners. Low vapor pressures are desired in products which should not change in bulk or dry out as in flexibilizers for glue, casein, etc., or plasticizers for lacquers or plastics.

SUBLIMATION

Sublimation is the direct vaporization of a solid that does not first liquefy; e.g., camphor or naphthalene.

Substances that sublime are useful when volatilization at certain temperatures is desired. Certain substances (camphor and naphthalene) sublime at ordinary temperatures. Of course, this means that the latter gradually disappears when exposed. Where such volatilization is undesirable, subliming substances should not be used.

BOILING POINT

The boiling point is the temperature at which the vapor pressure of a liquid equals the atmospheric pressure. Pure liquids have a definite boiling point. Commercial products, which contain impurities, boil over a range of temperatures, known as the boiling range. Thus, pure water boils at 100 C at 760 mm pressure. Commercial methyl oleate boils at 200-215 C at 15 mm pressure.

Low boiling liquids volatilize readily and disappear. This, of course, is advantageous where quick drying is necessary, as in the case of rubber cement or hair lacquers. High boiling liquids are specified where volatility is to be kept at a minimum to prevent drying out, brittleness, shrinkage, etc., as in the use of glycerin in Cellophane or castor oil in ethyl cellulose.

Boiling points can be varied by dissolving soluble materials in a liquid or by mixing it with another liquid of a different boiling point. In the former instance, the boiling point is raised whereas in the latter it is either lowered or raised, depending on the boiling point and solubility of the added liquid.