Using solubility parameters in cosmetics formulation

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Synopsis

This paper reviews the evolution of solubility theory from the basic concept to the current applied technology and provides several examples of its utility as applied to cosmetic materials and formulations. Solubility parameters of over 150 common cosmetic materials are reported, and the methods for calculating solubility parameters are presented along with an original, BASIC computer program utilizing Hildebrand's method.

INTRODUCTION

The goal of this research was to develop a method to evaluate and predict solubility interactions of cosmetic materials in formulations.

Understanding the forces and mechanics of solubility is a basic requirement for the scientific approach to cosmetic product formulation. Over the past decade remarkable advances have been achieved in the theory of liquids and in the prediction of physicochemical parameters of mixtures (1). The concept of the solubility parameter has been increasingly utilized by the coatings, drug, lubricant, and textile industries. The solubility parameter is described in recent textbooks and handbooks and can even be found in copy for advertising brochures of raw materials. Its application to cosmetics formulation is both timely and appropriate.

HISTORICAL BACKGROUND

Joel Hildebrand established the thermodynamic principles of intermolecular cohesion in 1936 (2). By 1950 he had defined the solubility parameter as the sum of all the intermolecular attractive forces, which he found to be empirically related to the extent of mutual solubility of many chemical species. Since Hildebrand's initial discoveries many other additions and refinements of the theory of "Cohesive Forces" (3–5) have facilitated application of the solubility parameter to problems of drug activity (6), polymer plasticization (7), pigment dispersion (8), solvent dyeing (9), adhesion (10), chromatographic separation (11), and many other challenges (12).

Recent advances in solubility theory have not only extended the scope but also improved the accuracy of calculations and predictions using solubility parameters. In general, the error of prediction does not exceed 10-20% (13). Concurrent with these improved methods, the advent of high pressure liquid chromatography (HPLC) and the decline

in microelectronic computational costs provided the way to impart a new impetus to the field of solubility research, especially dealing with non-electrolytes in non-aqueous systems. This area of research has so far produced three 1985 American Chemical Society Divisional Awards for excellence (14-16).

The use of computers (17) can improve the effectiveness and accuracy of the empirical method in all areas of formulation.

THEORY

The forces which cause materials to dissolve are the same forces which prevent a material from boiling away until a specific temperature is reached and which result in other physical characteristics we know such as viscosity. These forces are essentially magnetic in nature. Hildebrand defined the solubility parameter (δ) as the sum of all the cohesive forces and the square root of the energy of vaporization.

$$\delta = (\Delta E v/V)^{1/2}$$

where V = molecular weight/density and ΔEv = heat of vaporization.

It is not surprising that fluorocarbons give us both aerosol propellants (easy boiling) and Teflon[®] type (non-stick) surfaces, since both these attributes are a result of low cohesive forces.

Cohesive forces are attractive forces that radiate from all matter. Materials with strong cohesive forces attract each other in preference to materials with weaker fields. Thus the salts, gums, humectants, and water in a lotion are attracted to each other and dissolve because they all have similarly strong cohesive forces. The emollient oils, however, have weak forces and cannot make the associations needed to dissolve. They coalesce to form discrete droplets separated from the water phase, providing a medium suitable for ingredients with similar weak forces such as fragrances, some preservatives, and the oil-soluble tails of the amphiphilic emulsifiers, the heads of which project back into the water phase from which the oils were excluded.

NON-POLAR ATTRACTIONS

The atomic attractions contributing to the solubility parameter are the Van der Waals forces (18). These forces were found to be caused by tiny magnetic fields produced when an electron orbits the nucleus of an atom. When atoms combine to form molecules, the atomic fields also combine to yield a molecular field. The non-polar component of this is named for London (19) who recognized that the sum of these atomic forces in a molecule is proportional to the square of the polarizability (a) and to the inverse of the sixth power of the separation (r).

$$\mathbf{U} = \mathbf{a}^2 / \mathbf{r}^6$$

Because these fields also cause the dispersion or bending of light as it passes through a substance, they became known as London dispersion forces. Their contribution to the solubility parameter is defined as:

$$\delta_{\rm D} = 2.24 + 53 {\rm X} - 58 {\rm X}^2 + 22 {\rm X}^3$$
 and ${\rm X} = ({\rm n}^2 - 1)({\rm n}^2 + 2)$

where n = refractive index.

Prausnitz and Blanks (20) have more accurately determined the London contribution to the solubility parameter by assigning a value equal to the complete solubility parameter of non-polar homomorphs (i.e. compounds with the same general structure but with no polar groups attached). The electrodynamics of light bending by the cohesive field forces is still too poorly understood to provide an accurate measure of solubility parameter based on refractive index.

POLAR ATTRACTIONS

Polarity was originally considered to be the result of a single phenomenon; however, many different causes for polarity emerged from the study of how materials respond to electric charges and fields. By 1930 Debye had discovered that polarity in a molecule produced an additional electromagnetic attractive force caused by elongation of the more spheric London field. This dipole-dipole attraction is calculated to be:

$$U_d = -2/3(u^4/r^6)(1/kT)$$

where u is the dipole moment, k is the Boltzmann constant, T is the Kelvin temperature, and r is the separation.

In addition, the dipole moment induces a polarization in its neighbors:

$$U_i = -2au^2/r^6$$

where a, u, and r = as before.

The combined effect of these field deformations was analyzed by Keesom (21) and they now bear his name. However, it was Boettcher (22) who defined the polar contribution to the solubility parameter using the dielectric constant (e) and the refractive index (n):

$$\delta_{\rm p} = [12108(e - 1)(n^2 + 2)u^2/V^2(2e + n^2)]^{\frac{1}{2}}$$

where u and V = as before.

This was simplified by Beerbower (23) to:

$$\delta_{\rm p} = 18.3 \,{\rm u}/{\rm (V)^{1/2}}$$

where u and V = as before.

Unfortunately, both methods have areas of imprecision, with the Beerbower equation showing greater precision with alcohols. Nonetheless, the inclusion of polar contributions in calculations using the solubility parameter was the singular technological advance which made the solubility parameter become an effective tool in the polymer and coatings industry. Diagrams such as the one shown in Figure 1 are commonly used in the coatings industry to determine the choice of solvent for any particular resin by comparison of both the polar and total solubility forces.

In particular, this graph (24) compares both dipole moment and hydrogen bonding to the solubility parameter to determine the best solvents for the subject resin. Potential solvents are located by their solubility parameter and hydrogen bond strength within the "soluble area."

ASSOCIATIVE ATTRACTIONS

Consideration of the effects of hydrogen bonding and acid-base interactions has improved the accuracy of solubility estimations based on solubility parameters. Martin,



Figure 1. Comparison of dipole moment and hydrogen bonding to the solubility parameter.

Wu, and Beerbower (25) have recently used this expanded approach to study the solubility of methylparaben in 35 different solvents, with relatively good success. Kamlet (26), on the other hand, claims that acid-base interactions are better explained through hydrogen bond strength than through classical electron-donating potentials.

The formula describing the hydrogen-bonded electromagnetic field deformations has not been adequately developed from a theoretical standpoint, and estimates of hydrogen bonding are commonly based on infra-red spectral shifts. It is important to note that all the field formulas are divided by the distance of molecular separation to the sixth power. This makes both the polar and non-polar attractions drop off drastically with molecular separation. As a result, both heat and dilution can cause dramatic changes in solvent potential.

EXPERIMENTAL

Solubility parameters may be used to estimate the co-solubility of two materials through simply assessing their proximity by inspection. For example: Methylparaben ($\delta = 11.98$) is quite soluble in butylene glycol ($\delta = 13.20$) and hexyl alcohol ($\delta = 10.50$), while Glycerin ($\delta = 16.26$) and butyl stearate ($\delta = 7.68$) are comparatively poor

solvents. Co-solubilizers may be identified by the medial location of their solubility parameters between two relatively immiscible materials. In this way isopropyl myristate ($\delta = 8.02$) functions as a well known coupling agent in wax systems, like lipsticks, which incorporate normally immiscible mineral oil/castor oil ($\delta = 7.09/8.90$) combinations. Truly, some creative combinations of non-solvents have been produced which together exhibit good solvency, while being ineffectual alone. One common example of this "synergism" is the ethyl ether/ethanol ($\delta = 7.37/12.55$) solvent combination for nitrocellulose ($\delta = 11.25$). Individually these two solvents exhibit poor solvency for nitrocellulose. On the other hand, reverse synergism is also recognized where solvent mixtures interact with each other.

The solubility of benzalphthalide was evaluated as an example of using solubility parameters to determine the best choice of solvent and to demonstrate both the value and limitations of the solubility parameter for this purpose. Benzalphthalide is a new UV absorber of interest as a potential sunscreen. It is polar enough to demonstrate the separate solubility effects of the solubility parameter and the field deformations caused by inductive polarization and/or hydrogen bonding. It was the test material of choice because its manufacturer (VanDyk & Co.) describes it as a material with "limited solubility." The majority of cosmetic materials are less polar than benzalphthalide and their solubilities may be determined primarily from the solubility parameter. As materials become more polar or more hydrogen bonded, the polar and hydrogen bonding forces expectedly contribute more to the solubility of that material.

Two methods were used to determine the levels of solubility in the subject solvents. For volatile solvents, excess benzalphthalide was stirred and then allowed to stand isothermally at 25 degrees C. overnight before the supernatent was dried to constant weight. For solvents of lower volatility, incremental additions of solute were stirred isothermally until saturation was observed.

Figure 2 represents the results of the solubility study plotted against solubility parameter.

Figure 3 shows the same results plotted with respect to solubility parameter and dielectric constant. Hydrogen bonding is believed to be responsible for any anomalous results in this plot. The dependence of solubility on the value of the solubility parameter is apparent from both graphs. However, the contribution of the polarity provides increased precision to estimates of solubility in other solvents and to evaluation of the solvating forces surrounding benzalphthalide. One may also determine the solubility parameter of benzalphthalide to be about 10.9 from these results. Solubility studies like this are the ultimate empirical method for determining a solubility parameter. Among the non-polar majority of cosmetic materials, the overwhelming contibutor to effects of solubility is the solubility parameter.

APPLICATIONS OF THE SOLUBILITY PARAMETER

The solubility parameter has been applied successfully in fields other than cosmetics and toiletries, yielding practical solutions to many problems. These solutions have, in turn, been used to develop new products and processes and to improve on old technology. All of the methods reviewed below may be applied to cosmetic systems without modification.



Figure 2. Results of the solubility study plotted against solubility parameter.

The petroleum lubricant industry, for example, discovered the root causes of "slip" and "oilyness" through use of the solubility parameter (27). This new understanding led directly to the development of novel, vastly improved lubricants. The concepts of "slip" and "oilyness" or "lubricity" are clearly important to cosmetic technology.

Solubility is of major importance in biochemical processes. In 1964 Hansch (28) showed that drug activity depended equally on the lipid solubility of the drug molecule as well as its chemical reactivity. No drug can be effective if it cannot reach the location where it must work. From this rationale, correlations with solubility parameters have proved useful for designing insecticides, formulating liquid dosage pharmaceuticals, and analyzing transport of molecules through biological tissues (29).

Wetting and dispersion of pigments by solvents was analyzed by solubility parameter (30) to yield the surprising conclusion that although dispersability was related to cohesion parameter, wettability was not. Instead, wettability was found to be independent of pigment type due to moisture normally found adsorbed on the surface of pigment particles.

Plasticizers and solvents for resins are now routinely chosen by their solubility parameter (31), and new effective solvent mixtures (some constructed exclusively from non-solvents) are easily constructed by use of the parameter (32).

Foam control can be understood using cohesion parameters. The activity of a surfactant



Figure 3. Results of the solubility study plotted with respect to solubility parameter and dielectric constant.

is greatly affected by its bulk solubility. As a result, the foaming or foam-suppressing capacity of a surfactant is readily indicated by solubility parameter. The thermal change in this effect has been demonstrated for sodium stearate and block polyoxyethylene copolymers (33). Both these materials foam at high temperature but suppress foam when cold.

Emulsion stabilization can be effected in a manner similar to the stabilization or destabilization of foams. Beerbower (34) has shown a method of pre-calculating the requirements for a "perfect" stable emulsion and claims to have used his method to produce stable asphalt emulsions without trial and error. In this method the solubility parameter of the hydrophobic or lipophilic tail of the sufactant is matched to the solubility parameter of the emulsified oil. In any case, the concept of cohesive forces explains the mechanics of surfactant action. As Schott (35) has recently shown, the solubility parameter offers a more effective method for assessing the activity of a surfactant than Griffin's HLB system. This is because the HLB system took only the molecular weights of the two parts of a surfactant into account, while the cohesive approach accounts for its actual attractive force regardless of molecular weight.

DETERMINING SOLUBILITY PARAMETER

Many methods have been developed for the determination of the solubility parameter, ranging from essentially theoretical calculations, such as the Hildebrand/Scatchard

equation, to totally empirical correlations, such as the Kauri-Butanol number conversion published by Sevestre (36). Siddiqui made a comparison of several methods utilizing structural group contributions to the solubility parameter of n-propyl acetate (37). These are methods where portions of a molecule are given values which contribute to the total solubility parameter of the whole molecule. Hildebrand's method was chosen for computation of solubility parameters in this paper because this method is widely accepted and easily applied. It relies on molecular weight, boiling point, and density data which are commonly available for many materials and yields values which are usually within the range of other treatments. Moreover, the conversion from the calculated heat of vaporization (ΔHv) is the standard because this is the value originally defined by Hildebrand as the solubility parameter. This method is also preferred because it uses physical properties determined at the same ambient conditions under which many predictions may be desired. Sometimes the boiling point and density or molecular weight are not available for a material of interest, and so some alternate methods drawn from the literature have been included although the accuracy of these alternatives may be limited.

From heat of vaporization (Δ Hv) (Scatchard) (38):

$$\delta = (\Delta H v)^{1/2}$$

From boiling point (Hildebrand) (39):

 $\delta = [23.7T_B + .02T_B^2 - 2950 - 1.986K^{\circ}/(MW/Density)]^{1/2}$

where $T_B = \text{boiling point} @ 760 \text{ mm and } K^\circ = \text{density measurement temperature Kelvin.}$

From thermal expansion (Burrell) (40):

$$\delta = (aT/B)^{1/2}$$

where B = compressibility, a = coefficient of thermal expansion, and T = temper-ature of liquid.

From surface tension (Lee) (41):

$$\delta = 4.1 (\gamma/V^{1/3})^{0.43}$$

where γ = surface tension and V = molecular weight/density.

From refractive index (Lawson): (42)

$$\delta = [C(n^2 - 1)/(n^2 + 2)]^{\frac{1}{2}}$$

where n is the refractive index and C is a constant.

From gas law correction constants (Van der Waals) (40):

$$\delta = 1.2 a^{1/2}/V$$

where a = Van der Waals constant and V = molecular weight/density.From aniline point-ASTM D611 (Francis) (43):

$$\delta = 10.6 - [(4R/1.8)(A + 460/V + 91.1)]^{1/2}$$

where A = aniline point and R = Boltzmann constant.

From Kauri-Butanol point (KB)-ASTM D1133 (Sevestre) (36):

 $\delta = .02 \text{ KB} + 7.0$

for KB > 35.

From GLC activity coefficients (Alessi) (13):

 $\ln X = V/RT[(\delta_{DS} - \delta_D)^2 + (1 - 2m)(\delta_{PS} - \delta_P)^2] + [(\ln V/V_S + (1 - V/V_S)]]$ where X = activity coefficient, m = structural constant, and S indicates solvent. From HLB (Beerbower) (33):

 $\delta = \{118/(54 - HLB)\} + 6.0$

CALCULATIONS AND TABLES

In the past, solubility parameters have not been commonly used in the cosmetics and toiletries industry for reasons of expedience. Using solubility parameters is a comparative technique. Ideally, when one would like to know the solubility or compatibility of two materials, one most easily compares their solubility parameters. A difference of <2.0 usually indicates mutual solubility, although polar forces and hydrogen bonding are known to greatly affect this span. A mathematical model has recently been published by Kamlet and Taft (44) which uses the solubility parameter combined with measures of polarity and hydrogen bonding as was graphically demonstrated herein. They call their approach "solvatochromic" and achieve excellent predictive results; however, their method requires prior determination of solubility parameter, polarity, and strength of hydrogen bonding. This is admittedly a severe limitation. A practical approach is to make an estimate of solubility based on inspection of a table of solubility parameters or to use such a table to help determine appropriate solvents to use in a limited solubility study. This approach, made with an awareness of polar and hydrogen-bonding groups, can be expected to yield results more accurate and more rapid than the predominant rule-of-thumb, "Like dissolves like." In the past, the rule-of-thumb has predominated as a matter of practicality. Neither was a body of solubility parameter values for cosmetic materials available nor was there an easy method for determining the solubility parameter from easily determined or readily available physical constants. Our work with solubility parameters addresses both the above needs. Below is a listing of a computer program which will operate on the IBM PC or the Apple Macintosh with Microsoft Basic or on the Radio Shack Color Computer. It will determine the total solubility parameter of any chemical material based on boiling point, molecular weight, and density at a given temperature. It uses Hildebrand's method, including the empirical adjustments for ketones, aldehydes, and alcohols. This is the most common method used in the literature. Boiling points must be converted from reduced pressure values to 760 mm before calculating. A convenient nomogram for this purpose may be found in many handbooks or you may consult the original reference (45). The computer program is written in BASIC.

SOLUBILITY PARAMETERS OF COSMETIC MATERIALS

The need for a body of calculated solubility parameters of cosmetic materials is addressed here. The following table of cosmetic chemicals is listed by CTFA nomenclature in

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10 'Solparam
20 CLS
30 PRINT"Solubility Parameters by Hildebrand's Method"
40 PRINT"Program by CHRIS VAUGHAN"
50 PRINT" copyrighted 1985"
60 FOR X = 220 TO 880 STEP 20
70 SOUND X.2:NEXT:CLS
80 INPUT":chemical name";C$
90 INPUT "Molecular Wt.":MW
100 INPUT"Boiling Pt. at 760 mm";BP
110 INPUT"Density";DEN
120 INPUT"at what temp":T
130 \text{ SOL} = ((23.7^{*}(BP + 273) + .02^{*}(BP + 273)^{2} - .2950) - (1.986^{*}(273 + T)))/
(MW/DEN)
140 SOL = SOL^5
150 PRINT" Is the Chemical an Alcohol(a), Ester(e), Ketone(k), or
Neither(n)?"
160 I\$ = INKEY\$
170 IF I\$ = "a" THEN SOL = SOL + 1.4
180 IF I\$ = "e" THEN SOL = SOL + .6
190 IF I$ = "k" THEN SOUND 1000 .4: IF BP>100 THEN SOL = SOL + .5
200 IF I$ = "n"THEN 220
210 IF I$ = " " THEN 160
220 PRINT"The Solubility Parameter of:";C$; " is ";SOL; " at ";T;"Degrees C."
230 PRINT: PRINT, "want a hardcopy?? (Y) or (N)"
240 A = INKEY : IF A = " " THEN 240
250 IF A$ = "y" THEN 260 ELSE 270
260 LPRINT "The Solubility Parameter of:";C$;" is ";SOL;" at "; T;"Degrees C."
270 GOTO 80
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Figure 4. Computer program in BASIC for solubility parameter calculations.
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order of increasing solubility parameter, grouping the co-soluble materials together. The values listed here were either calculated by the BASIC computer program or taken from other literature(*). The physical constant data used to make the computations were taken from various handbooks, journal references, tables, and supplier's data sheets, or were supplied to the author by individual request. As such, they are subject to error and variation. For this reason we have cross referenced these computed results with other published solubility parameters where they exist and evaluated these results for compliance with general trends of structure/function. Several trends are readily evident from inspection, such as the uniform reduction of cohesive strength by increased branching or progressive chain length. However, some exceptions were substantiated by several sources. These have been retained in the table.

CONCLUSION

Solubility parameters can operate as an effective tool for the cosmetic chemist by shedding light on the most basic process in formulation, intermolecular cohesion. This is the force which gives stability and compatibility to products and packaging that are required by today's sophisticated consumer. It is also the same force which controls

CTFA Material Name	δ
Propellant 13	2.59*
Methane	4.70*
Cyclomethicone D5	5.77
Dimethicone	5.92*
Cyclomethicone D4	5.99
Squalane	6.03
Propellant 12	6.11*
Hexamethyldisiloxane	6.15
Squalene	6.19
Propane	6.21*
Propellant 22	6.23
Neopentane	6.38
Isopentane	6.82
Pristane	6.85
C8-Isoparaffin	6.93
White Mineral Oil	7.09*
Sperm Oil	7.09*
Pentane	7.10*
Hexane	.7.28
Linseed Oil	7.29*
Petrolatum	7.33*
Behenic Acid	7.35
Diethyl ether	7.37
Heptane	7.41
Octyl Palmitate	7.44
Propellant 11	7.49
Erucic Acid	7.57
Octane	7.58
Decane	7.62
C12-15 Alcohols Benzoate	7.63
Isobutyl Stearate	7.65
Butyl Stearate	7.68
Stearic Acid	7.74
Dioctyl Maleate	7.75
Isopropyl Palmitate	7.78
Oleth-3	7.83*
Linolenic Acid	7.86
Olive Oil	7.87*
Palmitic Acid	7.89
Oleic Acid	7.91
PEG-4 Stearate	7.92*
Isopropyl Myristate	8.02
Turpentine (pinene)	8.03
Methyl Oleate	8.05
Cetyl Acetate	8.06
Isostearic Acid	8.09
Myristic Acid	8.10
Melissyl Alcohol	8.22
Glyceryl Stearate (mono)	8.31*
Lauric Acid	8.46
Diisopropyl Adipate	8.46
Polyethylene	8.50*
Diisopropyl Amine	8.51*

 Table I

 Solubility Parameters of Some Cosmetic Materials

Purchased for the exclusive use of nofirst nolast (unknown) From: SCC Media Library & Resource Center (library.scconline.org)

CTFA Material Name	δ
Ethylene/Vinyl Acetate Copolymer (AC400)	8.55*
Sorbitan Laurate	8.61
Behenyl Alcohol	8.63
Isostearyl Alcohol	8.67
Zinc Stearate	8.80*
Citronellal	8.83
Oxidized Polyethylene (AC629)	8.85*
Methyl Isobutyl Ketone	8.85
Capric Acid	8.88
Muscone	8.89
Arachidyl Alcohol	8.89
Elaidyl Alcohol	8.90
Pentaerythritol Rosinate	8.90*
Stearyl Alcohol	8.90
B-Ionone	8.90
Dioctyl Phthalate	8.90*
Castor Oil	8.90*
Oleth-10	8.90*
Octyl Dodecanol	8.92
Butyl Acetate	8.93
Cetyl Alcohol	8.94
Oleyl Alcohol	8.95
Octyl Dimethyl PABA	9.01
Propyl Acetate	9.02
Glyceryl Laurate	9.08
Ceteth-20	9.10*
PPG-3 Methyl Ether	9.10*
Myristyl Alcohol	9.16
Ethyl Acetate	9.19
Methoxypropanol Acetate	9.20*
Sodium Stearate	9.29*
Citral	9.34
Caprylic Acid	9.35
Ethoxyethanol Acetate	9.40*
Isocetyl Alcohol	9.47
Nonylphenol	9.49*
Oxidized Polyethylene (AC392)	9.50*
Lauryl Alcohol	9.51
Ethylene/Vinyl Acetate Copolymer (AC430)	9.55*
Methylene Chloride	9.55
Cholesterol	9.55
PPG-2 Methyl Ether	9.60*
Undecyl Alcohol	9.61
MEK	9.63
Decyl Alcohol	9.78
Acetone	9.87
Dibutyl Phthalate	9.88*
Ethoxyethanol	9.90*
Caproic Acid	9.94
Tributyrin	9.97
Butoxy Diglycol	9.98*
Caprylic Alcohol	10.09
Geraniol	10.21
Butyl Lactate	10.27
t-Butyl Alcohol	10.28

Table I (continued)

Purchased for the exclusive use of nofirst nolast (unknown) From: SCC Media Library & Resource Center (library.scconline.org)

CTFA Material Name	δ
Pyridine	10.30
Methoxypropanol	10.40*
Isopropyl Lactate	10.42
Acetic Acid	10.42*
Nonoxynol-1	10.47*
Hexyl Alcohol	10.50
Butoxyethanol	10.53
Butylparaben	10.57*
Methyl Salicylate	10.62
Diacetone Alcohol	10.66
Triacetin	10.77
Methoxyethanol	10.80*
Ethyl Lactate	10.84
Benzalphthalide	10.90*
Benzaldehyde	11.00
D&C Red No. 22 (Eosin)	11.15*
Butyl Alcohol	11.18
Isopropyl Alcohol	11.24
Nitrocellulose	11.25*
PEG-8	11.34
Panthenol	11.39
PEG-6	11.47
Methyl Lactate	11.47
Benzoic Acid	11.50*
PEG-5	11.54
PEG-4	11.61
Acetonitrile	11.70
Propyl Alcohol	11.73
Phenethyl Alcohol	11.79
Phenoxyethanol	11.87
Sorbic Acid	11.97
Methylparaben	11.98
Triethylene Glycol	12.21
Benzyl Alcohol	12.31
Hexylene Glycol	12.32*
BHA	12.37
Alcohol	12.55
Adipic Acid	13.04
Butylene Glycol	13.20
Triethanolamine	13.28
Propylene Carbonate	13.35*
Dimethyl Sulfoxide	13.40
Diethylene Glycol	13.61
Propylene Glycol	14.00
Sodium Lauryl Sulfate	14.18*
Methyl Alcohol	14.33
Ethylene Glycol	14.50
Lactic Acid	14.81
PABA	14.82*
Ethanolamine	15.41*
Sodium Capryl Sulfate	15.80*
Glycerin	16.26
Ammonia	18.08
Water	23.40

Table I (continued)

most product properties, such as viscosity, volatility, lubricity, and tack, which give all cosmetics and toiletries their aesthetic appeal.

It is evident that the limits of precision achieved by solubility technology offer considerable opportunity for refinement. Nevertheless, this field has progressed to the point where it now can yield major contributions to the advancement of the level of scientific formulation. Because solubility parameters are based on thermodynamic principles, they will serve to show what can be possible given adequate kinetic (mixing) treatment.

Finally, the applicability of solubility parameters within the field of cosmetic chemistry has been demonstrated. Solubility parameters, unlike other measures of solubility, describe the physical size and strength of the intermolecular attractive fields. Therefore they lend themselves to mechanical explanations of intermolecular phenomena. As seen most recently in molecular biology, mechanical explanations can revolutionize a scientific field. Thus it is reasonable to expect many future refinements and computer applications of the solubility parameter applied to cosmetic chemistry.

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