

# POLYMER HANDBOOK

FOURTH EDITION

Editors

**J. BRANDRUP, E. H. IMMERMUT, and E. A. GRULKE**

Associate Editors

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# Solubility Parameter Values

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## A. INTRODUCTION

Applications of solubility parameters include selecting compatible solvents for coating resins, predicting the swelling of cured elastomers by solvents, estimating solvent vapor pressure in polymer solutions for devolatilization and reaction systems (16), and predicting phase equilibria for polymer–polymer (107), polymer–binary (93), random copolymer (102), and multicomponent solvents (38, 98,108,109).

Cohesive energy density and solubility parameters are defined in the section on miscibility of solvents and polymers (Section B). In addition, the applicability of solubility parameters to thermodynamic calculations and their limitations are discussed. Section C contains methods for measuring, calculating and correlating solubility parameters of solvents and polymers. Section D contains

alphabetical listings of solubility parameters (Table 7), a list of solubility parameters in rank order (Table 8), a list of three-component solubility parameters of solvents (Table 9), and a list of solubility parameters of polymers (Table 10). With the exception of Table 7, solubility parameter values are reported in MPa<sup>1/2</sup> units. The table showing solubility parameter value ranges for polymers (Table 3.4 in the third edition) has not been reproduced here.

## B. MISCIBILITY OF SOLVENTS AND POLYMERS

### 1. Cohesive Energy Density and the Solubility (Hildebrand) Parameter

Dissolution of an amorphous polymer in a solvent is governed by the free energy of mixing

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (B1)$$

where  $\Delta G_m$  is the Gibbs free energy change on mixing,  $\Delta H_m$  is the enthalpy change on mixing,  $T$  the absolute temperature, and  $\Delta S_m$  is the entropy change on mixing. A negative value of the free energy change on mixing means that the mixing process will occur spontaneously. Otherwise, two or more phases result from the mixing process. Since the dissolution of a high molecular weight polymer is always connected with a small or modest increase in entropy, the enthalpy term (the sign and magnitude of  $\Delta H_m$ ) is the deciding factor in determining the sign of the Gibbs free energy change. Solubility parameters were developed to describe the enthalpy of mixing of simple liquids (nonpolar, nonassociating solvents), but have been extended to polar solvents and polymers.

Hildebrand and Scott (59) and Scatchard (101) proposed that

$$\Delta H_m = V \left( \left( \frac{\Delta E_1^v}{V_1} \right)^{1/2} - \left( \frac{\Delta E_2^v}{V_2} \right)^{1/2} \right)^2 \phi_1 \phi_2 \quad (B2)$$

where  $V$  is the volume of the mixture,  $\Delta E_i^v$  the energy of vaporization of species  $i$ ,  $V_i$  the molar volume of species  $i$ , and  $\phi_i$  the volume fraction of  $i$  in the mixture.  $\Delta E_i^v$  is the energy change upon isothermal vaporization of the saturated liquid to the ideal gas state at infinite volume (94). The cohesive energy density (CED),  $\Delta E_i^v$ , is the energy of vaporization per cm<sup>3</sup>. The solubility parameter has been defined as the square root of the cohesive energy density and describes the attractive strength between molecules of the material.

$$\delta_i = \left( \frac{\Delta E_i^v}{V_i} \right)^{1/2} \quad (B3)$$

The dimensions of  $\delta_i$  are

$$\begin{aligned} (\text{cal/cm}^3)^{1/2} &= (4.187 \text{ J}/10^{-6} \text{ m}^3)^{1/2} \\ &= 2.046 \times 10^3 (\text{J/m}^3)^{1/2} = 2.046 \text{ MPa}^{1/2} \end{aligned} \quad (B4)$$

solvent (9–11).  $\delta_i$  is called the Hildebrand parameter by some authors. Other researchers (13) prefer the term, “cohesion parameter”, since it correlates with a large number of physical and chemical properties, and not just the miscibility of the components. The solubility parameter of a mixture is often taken as the sum of the products of the component solubility parameters with their volume fractions:

$$\delta_{\text{mixture}} = \sum_i \delta_i \phi_i \quad (B5)$$

### Relation between $\delta_i$ and $\Delta H_m$

Equation (B2) can be rewritten to give the heat of mixing per unit volume for a binary mixture:

$$\frac{\Delta H_m}{V} = (\delta_1 - \delta_2)^2 \phi_1 \phi_2 \quad (B6)$$

Equation (B6) gives the heat of mixing of regular solutions in which the components mix with: (a) no volume change on mixing at constant pressure, (b) no reaction between the components, and (c) no complex formation or special associations (114). The heat of mixing must be smaller than the entropic term in Eq. (B1) for polymer–solvent miscibility ( $\Delta G_m \leq 0$ ). When  $\delta_1 = \delta_2$ , the free energy of mixing will always be less than zero for regular solutions and the components will be miscible in all proportions. In general, the solubility parameter difference,  $(\delta_1 - \delta_2)$  must be small for miscibility over the entire volume fraction range.

**Relation between  $\delta_i$  and  $\Delta H_i^v$**  The energy change on isothermal vaporization can be related to the enthalpy of vaporization:

$$\Delta E_i^v = \Delta H_i^v + \Delta H_i^\infty - RT + p_i^s V_i \quad (B7)$$

where  $\Delta H_i^v$  is the enthalpy of vaporization at standard conditions,  $\Delta H_i^\infty$  the molar increase in enthalpy on isothermally expanding the saturated vapor to zero pressure,  $R$  the ideal gas constant, and  $p_i^s$  the saturation vapor pressure at temperature,  $T$ . At pressures below 1 atm, the  $\Delta H_i^\infty$  and  $p_i^s V_i$  terms are usually much less than the  $\Delta H_i^v$  and  $RT$  terms, and Eq. (B7) reduces to Eq. (B8):

$$\Delta E_i^v = \Delta H_i^v - RT \quad (B8)$$

The solubility parameter of volatile materials (solvents for example) can be determined by measuring their enthalpy of vaporization or using a correlation for this quantity, and using Eq. (B9):

$$\delta_i = \left( \frac{\Delta H_i^v - RT}{V_i} \right)^{1/2} \quad (B9)$$

Equation (B9) should be used at pressures near 1 atm. Near the critical point,  $\Delta H_i^v = 0$ , and Eq. (B8) incorrectly

predicts a negative value for the cohesive energy density while Eq. (B7) yields a small positive value.

**Dissolution of crystalline polymers** The free energy of mixing for crystalline polymers contains terms for the free energy of fusion for the crystalline volume fraction of the material. The free energy of fusion may contain terms that account for the loss of crystallite surface area and the mixing of amorphous material with oriented material. These terms would be added to Eq. (B1). The enthalpy of mixing could still be modeled using Eqs. (B2) or (B6). Some crystalline polymers obey the solubility parameter model at temperatures near their melting point,  $T > 0.9T_m$  (123). Solvent swelling experiments with crystalline polymers may fit Eq. (B1), particularly if the solvent is a poor one for the polymer and does not significantly dissolve crystalline regions.

### 2. Cohesive Energy Parameters for Polar Systems

The solubility parameter describes well the enthalpy change on mixing of nonpolar solvents but does not always give reliable results when extended to polar systems. The free energy change of mixing for polar systems is dominated by hydrogen-bonding forces between various groups in the solvent and polymer. Hydrogen-bonding forces are much stronger than van der Waals or dipole forces and often dominate the free energy of mixing. Complete miscibility is expected to occur if the solubility parameters are similar and the degree of hydrogen bonding (p: poor, m: moderate and s: strong) is similar between the components. Hydrocarbons, chlorinated hydrocarbons and nitrohydrocarbons are considered to be poor hydrogen-bonding solvents. Ketones, esters, and glycol monoethers give moderate hydrogen bonding. Alcohols, amines, acids, amides and aldehydes are strong hydrogen-bonding solvents. Table 7 classifies materials using these categories (21–24). Alternative classifications have been given by Lieberman (69), Gardon (41,85,86) and Dyck and Hoyer (32).

Other investigators have decomposed the Hildebrand parameter into several terms representing different contributions to the free energy of mixing. Hildebrand (59) used dispersive and polar solubility terms for solvents, with the complete parameter being given by

$$\delta^2 = \delta_d^2 + \delta_p^2 \quad (B10)$$

where  $\delta_d$  is the dispersive term and  $\delta_p$  the polar term. The additional term improved agreement between  $\delta$  and experimental data. Prausnitz and coworkers accounted for polar bonding by including parameters for permanent dipole interactions and dispersion type interactions. This approach has been applied to polymer solutions (15) and complex formation (57). Crowley et al. (26,27) proposed a three-parameter system.

Hansen (49–53,56) and Hansen and Skaarup (54) assume that the cohesive energy arises from dispersive,

permanent dipole–dipole interactions and hydrogen bonding forces:

$$\delta^2 = \delta_d^2 + \delta_p^2 + \delta_h^2 \quad (B11)$$

where  $\delta_h$  accounts for a variety of association bonds, including hydrogen bonds and permanent dipole-induced dipole (47). The values of these components for solvents were calculated from a large number of solubility data sets. Polymer solubility parameters can also be decomposed to a three-term set. The Hansen parameters give improved agreement with data but are still not completely accurate in predicting solutions thermodynamics for every system. Peiffer (172) has related dispersion, polar and induced solubility parameters to intermolecular forces and molecular size. The dispersive component increases with molecular size, while the polar component decreases with molecular size.

**Temperature effects** The solubility parameter decreases with temperature. The individual terms have varied dependence on temperature, namely (Ref. 55)

$$\begin{aligned} \frac{d\delta_d}{dT} &= -1.25 \times \alpha \times \delta_d \\ \frac{d\delta_p}{dT} &= -\frac{\delta_p \times \alpha}{2} \\ \frac{d\delta_p}{dT} &= -\delta_h \left( 1.22 \times 10^{-3} + \frac{\alpha}{2} \right) \end{aligned} \quad (B12)$$

where  $\alpha(K^{-1})$  is the volumetric thermal expansion coefficient.

### 3. Relationship between Solubility Parameters and other Thermodynamic Parameters

Hildebrand and Hansen parameters can be calculated using other thermodynamic quantities. This section contains some of the relationships for binary systems. Extensions to multicomponent systems are described by Flory (37) and Olabisi et al. (89).

**Activity coefficients** Excess free energy calculations for regular solutions (93) can be used to relate solubility parameters and solvent activity coefficients:

$$RT \ln \gamma_1 = V_1 \phi_2^2 (\delta_1 - \delta_2)^2 \quad (B13)$$

$$RT \ln \gamma_2 = V_2 \phi_1^2 (\delta_1 - \delta_2)^2 \quad (B14)$$

where  $\gamma_i$  is the activity coefficient of component  $i$ . Equations (B13) and (B14) depend on the use of the geometric mean,  $\delta_{12} = (\delta_1 \times \delta_2)^{1/2}$ . Funk and Prausnitz (40) show that there are deviations from this rule for aromatic hydrocarbons.

**Molar excess free energy of mixing** The molar excess free energy of mixing for binary solutions is

$$\Delta G^E = \sum_i (\delta_{1-i} - \delta_{2-i})^2 \quad (B15)$$

where  $\delta_{j-i}$  is the solubility term of group  $i$  for species  $j$ .

**Polymer-solvent interaction parameter** The polymer-solvent interaction parameter,  $\chi$ , is modeled as the sum of entropic and enthalpic components:

$$\chi = \chi_H + \chi_S \quad (B16)$$

where  $\chi_H$  is the enthalpic component and  $\chi_S$  is the entropic component.  $\chi_S$  is usually taken to be a constant between 0.3 and 0.4 for nonpolar systems:  $\chi_S = 0.34$  is often used (15,104). The enthalpic component can be related to the Hildebrand parameters:

$$\chi_H = \frac{V_1}{RT} (\delta_1 - \delta_2)^2 \quad (B17)$$

Substituting Eq. (B17) into Eq. (B16)

$$\chi = \frac{V_1}{RT} (\delta_1 - \delta_2)^2 + 0.34 \quad (B18)$$

Equation (B18) permits only positive values of the interaction parameter. Since the Flory-Huggins criterion for complete solvent-polymer miscibility is  $\chi < 0.5$ , the enthalpic contribution must be small and the solubility parameters of the solvent and polymer must be similar (21). The molar volume of the solvent also affects miscibility and phase equilibria: a Hildebrand parameter needed for phase separation or miscibility cannot be specified without specifying  $V_1$ .

**Interchange energy density** Equation (B18) works well for nonpolar systems for which Eq. (B17) is a good description of the enthalpic component of the interaction parameter. The geometric mean assumption of regular solution theory is not appropriate for polar systems, and better models include an extra term describing the interchange energy density for the solvent-polymer pair. For example

$$\chi = \chi_S + \frac{V_1 A_{12}}{RT} \quad (B19)$$

with

$$A_{12} = \delta_1^2 + \delta_2^2 - 2 \times l_{12} \delta_1 \delta_2 \quad (B20)$$

where  $l_{12}$  characterizes the intermolecular forces between molecules (rather than using the geometric mean assumption). Equation (B20) allows the modeling of specific interactions between components 1 and 2. Mixed solvents can be treated as a single solvent by determining the solubility parameter of the solvent mixture, and then using this value in Eq. (B18). If both the solvents and the polymers interact, the description is more complicated. An alternative definition of  $A_{12}$  uses the two-component solubility parameter (Ref. 25)

$$A_{12} = (\delta_{1d} - \delta_{2d})^2 + (\delta_{1p} - \delta_{2p})^2 \quad (B21)$$

The Hansen parameters may also be used to model  $A_{12}$ .

Several recent theories for polymer solution thermodynamics include entropic, enthalpic and free-volume contributions to the free energy of mixing. The free-volume contributions modify the entropic components, and have the opposite temperature dependence from the combinatorial term, helping to explain the lower critical solution temperature. Since Eq. (B18) assumes a constant value for the entropic component, it may not be valid over large temperature ranges. However, Eq. (B18) will predict the upper critical solution temperature, and, from this standpoint, is adequate for a number of phase equilibria applications near this condition.

The Lattice Fluid model (170) can be used to predict the solubilities of hydrocarbon and chlorinated hydrocarbons in nonpolar polymers. Three-dimensional solubility parameters can be used to provide an empirical correction to the geometric mean approximation (171). This correction predicts the solubility of polar and nonpolar solvents in polymers using only the pure component equation-of-state and solubility parameters.

**Guide to polymer-solvent miscibility** A region of solubility has been characterized by the distance between solvent and solute coordinates (Ref. 14)

$$R_{ij} = \left( 4(\delta_{1d} - \delta_{2d})^2 + (\delta_{1p} - \delta_{2p})^2 + (\delta_{1h} - \delta_{2h})^2 \right)^{1/2} \quad (B22)$$

A more general definition of the region of solubility is

$$R_{ij} = \delta_1 - \delta_2 = (a(\delta_{1d} - \delta_{2d})^2 + b(\delta_{1p} - \delta_{2p})^2 + b(\delta_{1h} - \delta_{2h})^2)^{1/2} \quad (B23)$$

where  $a$  and  $b$  are empirical weighing factors. If the distance between the solvent and the solute Hansen coordinate position exceeds  $R_{ij}$ , the two components are not soluble, or swelling is less than expected.  $R_{ij}$  reduces the need for three-dimensional plots. Some investigators have used two-dimensional plots for polar and hydrogen bonding terms, but the technique may be misleading for materials with large dispersion contributions. Barton (12) gives a number of models and contour map examples. As mentioned previously, Eqs. (B17)–(B19) suggest that the solvent molar volume can have a significant effect on miscibility.

Zeller (131) reviewed graphical three-dimensional solubility parameter estimation methods (12,14,49,55,172,173) as applied to solvent swelling of crosslinked elastomers. In general, the graphical method (Eqs. B22 and B23) does not account for the known influence of molar volume and crosslink density of solubility, and incorrectly assumes a linear relationship between the solubility parameter difference and solubility. An improved method used the Flory-Rehner equation to modify the interaction parameter for the effects of crosslink density (132).

**Guide to polymer-polymer miscibility** In many polymer-polymer systems, miscibility can be predicted by comparing the solubility parameters (139). The following table proposes miscibility guidelines. Polymer-polymer miscibility is enhanced when hydrogen bonding is present.

TABLE OF MISCELLITY GUIDELINES<sup>a</sup>

Intermolecular interaction	Polymer blend example	Critical value of the interaction parameter, $\chi_{crit}$	Upper limit of the non-hydrogen bonded solubility parameter difference, $\Delta\delta$ (MPa <sup>1/2</sup> )
Dispersive forces only	Polyisoprene-Poly(vinylethylene)	<0.002	<0.02
Dipole-dipole interactions	Poly(methyl methacrylate)-poly(ethylene oxide)	0.002–0.001	0.2–1.0
Weak hydrogen bonds	Poly(vinyl chloride)-polycaprolactone	0.02–0.2	1.0–2.0
Moderate hydrogen bonds	Poly(vinyl phenol)-poly(vinyl acetate)	0.2–1.0	2.0–5.0
Strong hydrogen bonds	Poly(vinyl phenol)-poly(vinyl methyl ether)	1.0–1.5	5.0–6.0

<sup>a</sup> Ref. 139.

### C. SOLUBILITY PARAMETER MEASUREMENTS, CALCULATIONS, AND CORRELATIONS

Solubility parameters can be determined by direct measurements, indirect calculations, or correlations with other physical parameters. The solubility parameters of solvents usually can be determined directly by measuring the energy of vaporization. The solubility parameters of polymers can only be determined indirectly and may be affected by variations in their chemical constitutions, i.e., the number of crosslinks and the distribution of chain branches or substitutive groups along the polymer backbone. The methods presented in this section can be used to develop correlations of solubility parameters with other physical properties for specific commercial polymer products or to estimate the solubility parameters of new polymers.

#### 1. Solvents

**Calculation of the solubility term ( $\delta$ ) by relating the enthalpy of vaporization to the energy of vaporization** Equation (B8) can be used to calculate  $\Delta E_i^v$  when  $\Delta H_i^v$  is available. The molar volume of the solute is needed to complete the calculation of  $\delta$ , using Eq. (B3). This is the most direct and accurate method of determining the solubility parameter. However,  $\delta$ 's determined in this way may not give the best prediction of solution behavior. The solubility parameter values in Tables 7–9 reflect the solvent's behavior in a variety of systems.

**Correlations** Both the enthalpy of vaporization and the molar volume of a solvent can be estimated from

correlations. When  $\Delta H_i^v$  is known at the normal boiling point, it can be converted to the appropriate value at a second temperature using (126)

$$\frac{\Delta H_i^v(T_2)}{\Delta H_i^v(T_1)} = \left( \frac{T_c - T_2}{T_c - T_1} \right)^{0.38} \quad (C1)$$

This corresponding state-type procedure gives estimates within 2% of experimental values over a wide range of temperatures (13). Hildebrand and Scott (59) proposed an empirical correlation between  $\Delta H_i^v$  at 25°C and the normal boiling point,  $T_b$ :

$$\Delta H_i^v(298K) = 0.2950 + 23.6 T_b + 0.020 T_b^2 \quad (C2)$$

with enthalpy units of kcal/mol. Lawson (67) suggests different coefficients to include fluorocarbon liquids. The Clausius-Clapeyron equation can be applied if vapor pressure data are available. Eq. (C2) is reasonably accurate only for liquids that are not hydrogen bonded. The Hildebrand parameter calculated by Eq. (C2) should be adjusted as follows for different solvents (24): add 1.4 (cal/cm<sup>3</sup>)<sup>1/2</sup> for alcohols, add 0.6 (cal/cm<sup>3</sup>)<sup>1/2</sup> for esters, and add 0.5 (cal/cm<sup>3</sup>)<sup>1/2</sup> for ketones if the boiling point is less than 100°C. Jayasri and Yaseen (64) suggest adding 1.7 (cal/cm<sup>3</sup>)<sup>1/2</sup> for alcohols.

Solvent molar volumes are available or can be calculated by group molar volume methods at 25°C (35,163–165). The molar volume for solids at 25°C can be extrapolated from liquid state values (the liquid is assumed to be subcooled).

**Thermodynamic coefficients** The internal pressure,  $\pi$ , is defined as (Ref. 88)

$$\pi = \frac{\partial E}{\partial V} = T\beta - P \quad (C3)$$

where  $\beta$  is the constant volume thermal pressure coefficient (the ratio of the coefficient of thermal expansion,  $\alpha$ , to the isothermal compressibility,  $\kappa$ ). Since the external pressure is usually small with respect to  $T\beta$ , the internal pressure is approximated by

$$\pi = T\beta = T \frac{\alpha}{\kappa} = T \left( \frac{\partial P}{\partial T} \right) \quad (C4)$$

The Hildebrand parameter is the square root of the internal pressure. Eq. (C4) provides a method for scaling the Hildebrand parameter with temperature. This equation also provides a method for the direct estimation for  $\delta$  of polymers;  $\alpha$  and  $\kappa$  are measurable when  $\Delta H_i^v$  is not meaningful (B7). The thermal pressure coefficient (C4) can be evaluated from vapor-pressure data and is easier to apply than the Clausius-Clapeyron equation. For high pressure membranes, the external pressure term in Eq. (C3) may not be negligible. Solubility parameters generally decrease with increasing pressure.

**van der Waals gas constant** Tables are available in many Handbooks for the van der Waals correction constants to the ideal gas law,  $a$  and  $b$ , where  $a$  has units of  $\text{l}^2/\text{atm}$ . For some liquids, these values may be at hand when other data are not available. They can be used to check Hildebrand parameter values obtained from other sources.

$$\delta = 1.2 \frac{\sqrt{a}}{V} \quad (\text{C5})$$

The form of Eq. (C5) can be obtained by substituting the van der Waals equation of state into Eq. (C3).

**Critical pressure** The solubility parameter is related to the critical pressure,  $P_c$  of a substance through the empirical equation

$$\delta = 1.25 P_c^{1/2} \quad (\text{C6})$$

where the critical pressure is expressed in atmospheres. Equation (C6) is not very accurate, but is simple to apply when critical pressure data are available.

**Surface tension** Michaels (83) has shown that the surface tension can be related to the cohesive energy density:

$$\frac{\Delta E_i}{V_i} = A \left( \frac{1}{V_i} \right)^{1/3} \gamma_L \quad (\text{C7})$$

where  $\gamma_L$  is the surface tension and  $A$  is a constant. Koenhen and Smolders (65) correlated surface tension and two Hansen parameters:

$$\delta_d^2 + \delta_p^2 = 13.8 \left( \frac{1}{V_i} \right)^{1/3} \gamma_L \quad (\text{C8})$$

$\delta_h$  is probably not related to the liquid-vapor interfacial energy as these interactions do not involve breaking hydrogen bonds. Eq. (C8) does not describe cyclic compound, acetonitrile, carboxylic acids, polyfunctional alcohols, and other polar compounds well. Hildebrand and Scott (59) have proposed a different equation, which has been discussed by Lee (68).

**Index of refraction** The dispersive Hansen parameter can be related to the index of refraction,  $n_D$  (65,105).

$$\delta_d = 9.55 n_D - 5.55 \quad (\text{C9})$$

The interaction energy between nonpolar molecules should depend on polarizability (London dispersion forces) and, therefore, on the index of refraction.

**Dipole moment** Hansen and Skaarup (54) related the polar Hansen parameter to the dielectric constant,  $\epsilon$ , and the dipole moment,  $\mu$ :

$$\delta_p^2 = \frac{12108}{V^2} \frac{\epsilon - 1}{2\epsilon + n_D^2} (n_D^2 + 2)\mu^2 \quad (\text{C10})$$

Beerbower and Dicky (14) proposed an empirical relationship:

$$\delta_p^2 = 9.5 \frac{\mu}{V_i^{1/2}} \quad (\text{C11})$$

**Kauri butanol values** Proprietary hydrocarbon solvents are usually mixtures with boiling ranges and unknown molecular weights. Solubility parameter values may be estimated from Kauri butanol values (ASTM Method D1133-54T) using the equation

$$\delta = 6.3 + 0.03 KB \quad (\text{C12})$$

## 2. Polymers

Hildebrand parameters cannot be calculated for polymers from heat of vaporization data because of their nonvolatility. Indirect methods are described below. The solubility parameter values in Table 10 may only be representative of a given polymer since variations in compositions can lead to changes in  $\delta$ .

### 2.1. Indirect Measurements

**Solvency testing (screening procedure)** The classic method for determining solubility parameter of a commercial polymer is solvency testing, or the solvency screening procedure. This technique compares polymer solubility in solvent groups with different hydrogen bonding characteristics (poor, moderate and strong). The midpoints of the polymer's solubility range may be used as single-valued quantities for some purposes, but may not agree with values determined by other methods (43). A gram or two of solid polymer is placed in a test tube and an approximate amount of a selected solvent is added such that the final solution would have about the correct solid content for the expected commercial use, e.g., 50% for alkyds, 20% for vinyls, etc. The exact amount is often unimportant, except for poor solvents. A typical phase diagram for binary polymer-solvent systems may show upper and lower critical solution temperatures. The one-phase region expands away from the UCST and LCST points, which often occur in the range of 20–80 wt.% polymer. The usual purpose of these experiments is to find good solvents for commercial product formulation, and this screening procedure will help identify such solvents. The mixture may be warmed and stirred to speed up solution, but it should be cooled and observed at room temperature. The resulting mixture should be a single phase, clear and free of gel particles or cloudiness; otherwise the polymer is judged insoluble. The solvents to be used are selected from Table 1.

This grouping of solvents has been selected so that the Hildebrand parameter values increase by reasonably constant steps within each hydrogen bonding class. The object of using these solvent spectra is to establish a solubility parameter range for a polymer rather than a single-valued number. This range has the advantage of showing the difference,  $(\delta_1 - \delta_2)^2$  (see Eqs. B13, B14 and

B18), which can be tolerated between the solubility values of the polymer and solvent for miscibility. Van Dyk et al. (120) have shown that the molar volume improves the correlation between solvency and the solubility parameters. A better measure of solubility might be the group,  $V_1(\delta_1 - \delta_2)^2$ .

In carrying out the procedure, it is convenient to select the first trials about 1/2 and 2/3 of the way down the column; for example, in the poorly hydrogen bonded group, toluene and nitroethane would be chosen. If the polymer is soluble in both, there is no need to try intermediate solvents because experience has shown that the polymer will be soluble in every case. The solvents at the end of the spectrum should be tried next. If the polymer is soluble in one but not both of the initial trials, the third trial should be half-way between the two. By successive choices, sets of two adjacent solvents will be found, one of which dissolves the polymer and one that does not. The parameter values of the solvents which do dissolve the polymer mark the ends of the range. The procedure is repeated for the other two hydrogen bonding classes.

**Osmotic pressure** Fedors (35) used the osmotic pressure of polymer solutions to determine solubility parameters.

**Swelling values** Another method for measuring the solubility parameter of polymers is to prepare a sparsely crosslinked sample and immerse it in a series of liquids of varying  $\delta$  (166,167). The crosslinked material will swell to varying degrees, with the maximum amount of swelling occurring when the solvent has the same Hildebrand parameter as the polymer. The amount of swelling can be measured by length, weight, or volume changes. By inference, the soluble, uncrosslinked materials has the same value. An example of a crosslinked sample is styrene polymerized with 1% divinyl benzene.

**Turbidity** Polymer can be precipitated from dilute solution by adding a non-solvent. The cloud point defines the onset of two phases. The enthalpic component of the interaction parameter,  $\chi_H$ , can be related to the solubility parameter difference between the solvent and the polymer (Eq. B17). Two different non-solvents are used: one having a solubility parameter above that of the solvent, and another having a solubility parameter below that of the solvent. The enthalpic components of the interaction parameter for each phase are equal at the cloud point, which can be used to measure the solubility parameter of the polymer (116). The two expressions for  $\chi_H$  are

$$\frac{V_{ml}(\delta_2 - \delta_{ml})^2}{RT} = \frac{V_{mh}(\delta_2 - \delta_{mh})^2}{RT} \quad (\text{C13})$$

where  $V_{ml}$  and  $V_{mh}$  represent the molar volumes at the cloud points of the solvent-lower solubility parameter nonsolvent and solvent-higher solubility parameter nonsolvent, respectively.  $\delta_{ml}$  and  $\delta_{mh}$  are the solubility

parameters of the mixed solvents. The mixture properties are calculated using

$$\delta_m = \phi_1 \delta_1 + \phi_3 \delta_3 \quad (\text{C14})$$

$$V_m = \frac{V_1 V_3}{\phi_1 V_3 + \phi_3 V_1} \quad (\text{C15})$$

where the subscripts, 1 and 3, refer to the solvent and the nonsolvent. Eq. (C13) is simplified to determine the solubility parameter of the polymer:

$$\delta_2 = \frac{(\sqrt{V_{ml}} \delta_{ml} + \sqrt{V_{mh}} \delta_{mh})}{(\sqrt{V_{ml}} + \sqrt{V_{mh}})} \quad (\text{C16})$$

The volume fraction of the nonsolvent at the cloud point is used to compute the solvent mixture solubility parameter and molar volume. Cloud point experiments are done for a series of solvents with the two nonsolvents, generating a set of points,  $(\delta_1, \delta_2)$ . The intersection of the line defined by this set of points with the line,  $\delta_1 = \delta_2$ , determines the polymer's solubility parameter.

**Specific volume** The specific volume of polymers varies with the solvent. Good solvents give higher values of the specific volume while poor solvents give lower values. A plot of the polymer specific volume as a function of solubility parameter gives a maximum value, which is taken to be the solubility parameter of the polymer. High precision density measurements at carefully controlled temperatures are needed for this method (168). The partial specific volume is defined as

$$\bar{V}_i = \frac{\partial V}{\partial c_i} \Big|_{T,p,i \neq j} \quad (\text{C17})$$

The specific volume of a nonideal two-component system is

$$V_{\text{spec}} = \phi_1 \bar{V}_1 + \phi_2 \bar{V}_2 \quad (\text{C18})$$

where  $\bar{V}_2$  is the rate of change in volume of the solution when a very small amount of polymer is added. As the solvent volume fraction goes to one, the partial molar volume of solvent is constant and Eq. (C18) becomes

$$V_{\text{spec}} = \bar{V}_{1(c_2=0)} + \phi_2 \bar{V}_2 \quad (\text{C19})$$

The maximum of the polymer partial specific volume is estimated by fitting a quadratic to the data (Ref. 142):

$$\bar{V}_2 = \bar{V}_{2,\max} - A(\delta_1 - \delta_2)^2 \quad (\text{C20})$$

It is possible to estimate the polymer solubility parameter with only two reference solvents (168), but more reliable values are found by using a range of solvents.

**Intrinsic viscosity** A number of researchers have used intrinsic viscosity to estimate Hildebrand parameters (74).

Flory (37) related intrinsic viscosity to polymer molecular weight and the chain-expansion factor. The chain-expansion factor can, in turn, be related to the polymer-solvent interaction parameter using the Flory-Huggins theory. Maximum coil extension should occur in solvents near the polymer's solubility parameter. A variety of models can be used to relate the interaction parameter to Hildebrand parameters (19,80,115,167-169). These equations are quadratic (Eq. C21) or take the form of a gaussian curve (Eq. C22):

$$[\eta] = [\eta]_{\max} - A(\delta_1 - \delta_2)^2 \quad (\text{C21})$$

$$[\eta] = [\eta]_{\max} \exp(-A(\delta_1 - \delta_2)^2) \quad (\text{C22})$$

where  $[\eta]$  is the intrinsic viscosity,  $[\eta]_{\max}$  the maximum intrinsic viscosity, and  $A$  the constant. These researchers have shown that Eq. (C14) gives a good correlation between solvency and Hansen parameters for methacrylate polymers.

**Inverse phase gas chromatography** This method has been used by a number of investigators to measure infinite dilution weight fraction activity coefficients (6,29-31,63,71,72,84,90,91,113). These coefficients can be related to Hildebrand parameters by using a thermodynamic theory for polymer solutions, such as Flory-Huggins theory. The polymer is the stationary phase in a gas chromatography column. Both binary and multicomponent equilibria (46,99,100) can be studied using this method. Chromatographic techniques have the advantage of rapid measurement of thermodynamic values once the columns have been made. The solubility parameter can be related to the specific retention volume of the solvent on the column. Both  $V_i$  and  $\Delta H_i^v$  must be known at the temperature of the column. Molar volumes for the solvents can be determined by using literature density equations or generating equations from density data. Values for the enthalpy of vaporization can be determined at the experimental temperature (71).

The inverse phase gas chromatography method has the advantage of providing values for the infinite dilution solubility parameter,  $\delta_i^\infty$ , over a range of temperatures. This is particularly valuable for the prediction of phase equilibria at elevated temperatures. The value of  $\delta_i^\infty$  at 25°C can be estimated by using the expected temperature dependence for  $\chi$  (Eq. B18) of

$$\chi = \alpha + \frac{\beta}{T} \quad (\text{C23})$$

One potential problem with this technique is that  $\chi$  is known to be a function of concentration and the polymer Hildebrand parameter is determined at infinite dilution of solvent. For a number of binary systems, the change in  $\chi$  with solvent weight fraction is the largest as  $\omega \rightarrow 0$ . The concentration dependence of the interaction parameter can be modeled using methods given in the chapter on interaction parameters in this Handbook.

## 2.2. Correlation Methods

**Refractive index** Koenhen and Smolders (65) have predicted dispersive Hansen parameters from refractive index measurements of polymers. Wu (128) has suggested an effective cross-sectional area to relate the cohesive energy density and surface tension

$$\delta_d^2 = A \left( \frac{n_s}{V_{i,s}} \right)^{1/3} \gamma_s^d \quad (\text{C24})$$

where  $n_s$  is the number of atoms in a segment,  $V_{i,s}$  the molar volume of a segment, and  $\gamma_s^d$  the dispersion contribution to the free surface energy of the polymer.

**Dipole moment** Equation (C10) has been applied to polymers by Koenhen and Smolders (65). The dipole moments of polymers are between 70% and 90% of those of the corresponding monomer units.

**Hydrogen-bonding parameter** Hansen and Beerbower (55) compiled enthalpy data for hydrogen bonding groups. The following values are suggested:

Group	Cohesive energy, $E_h$ , (kJ/mol)	Refs.
Alcohol	20.9	-
Amide	16.3	83
Ester	5.2	54
Nitrile	2.1	54
Ether	2.3	54
Monochloro substituent	0.4	54
Phenylene ring	0.4	54

The hydrogen-bonding parameter is given by

$$\delta_h^2 = \frac{E_h}{V_i} \quad (\text{C25})$$

**Group contribution methods** These methods have been used to estimate the solubility parameter (17,20,28,33,35, 58,60,61,96,112,121,122), van Krevelen (123), Fedors (35), and Barton (12) have reviewed these techniques and given tables of group values. The molar volume of solvents and polymers can also be estimated by group contribution techniques (108).

The sets of group constants of Small (112), Hoy (61) van Krevelen (121) and van Krevelen and Hoftyzer (122) seem to be most comprehensive. Table 2 gives the group molar attraction constants at 25°C. Small's values were derived from measurements of the heat of vaporization. Hoy's values were derived from vapor pressure measurements. The group contribution values of van Krevelen and Hoftyzer are based on cohesive energy data of polymers.

The group contribution techniques are based on the assumption that the contributions of different functional groups to the thermodynamic property are additive. The energy of vaporization of a solvent or polymer is

$$\Delta E_i^v = \sum_j n_j \Delta e_j \quad (\text{C26})$$

where  $\Delta e_j$  is the energy of vaporization contribution of group  $j$ , and  $n_j$  the number of groups of type  $j$  in the molecule. The solubility parameter is obtained by combining Eqs. (B3) and (C26):

$$\delta_i = \left( \frac{\Delta E_i^v}{V_i} \right)^{1/2} = \left( \frac{\sum_j n_j \Delta e_j}{V_i} \right)^{1/2} \quad (\text{C27})$$

Small (112) defined the molar attraction constant as

$$F_j = (\Delta E_{i,j}^v V_{i,j})^{1/2} \quad (\text{C28})$$

that can be used to calculate the solubility parameter by

$$\delta_i = \left( \frac{\Delta E_i^v V_i}{V_i^2} \right)^{1/2} = \frac{\sum_j F_j}{V_i} = \frac{\rho_i \sum_j F_j}{M_i} \quad (\text{C29})$$

where  $\rho_i$  is the polymer density and  $M_i$  is the polymer molecular weight.  $\delta_i$  can be evaluated for polymer repeating group by using group contribution calculations for the molar volume and the cohesive energy density or molar attraction constant. Table 2 gives sets of molar attraction constants and the energy of vaporization provided by several different authors. It is preferable to use parameters from only one set when determining the solubility parameter of a repeating unit. Table 3 gives the cohesive energy densities and group molar volumes determined by Fedors. This set may give less accurate estimates than those in Table 2, but it has value because it is more comprehensive and can be applied to more systems.

**Hansen parameters** The terms in Eq. (B11) can be estimated by group contribution methods. In general, the resulting factors are known less accurately than the group molar attraction constants or energy of vaporizations. The interaction of structural groups within molecules may not follow simple additive rules. However, the estimate of Hansen parameters can be very useful. Under the method of Hoftyzer and van Krevelen (Table 4), the terms are estimated as

$$\delta_d = \frac{\sum F_{di}}{V} \quad (\text{C30})$$

$$\delta_p = \sqrt{\frac{\sum F_{pi}^2}{V}}$$

$$\delta_h = \sqrt{\frac{\sum E_{hi}}{V}}$$

The dispersive Hansen parameter treats the molar attraction constants as additive. The polar Hansen parameters also are additive, unless more than one polar group is present. Methods for treating additional polar groups are given in

the last three rows of Table 4: additional polar groups do not add linearly to the polar Hansen term. The molar attraction constant is not applied to the hydrogen-bonding Hansen parameter. Rather, a hydrogen bonding energy,  $E_{hi}$ , is used.

Hoy (178-179) has an alternative group contribution method (Table 5). It includes a molar attraction function,  $F_{t,i}$  a polar component of this function,  $F_{p,i}$ , the molar volume of the solvent or polymer structural unit, the Lyderson correction for solvent non-ideality,  $\Delta_{T,i}$ , and a similar correction for polymer non-ideality,  $\Delta_{T,i}^{(P)}$ .

Bicerano (164) and Porter (165) have developed new group contribution techniques for a wide variety of polymer properties. These approaches consider how the different functional groups are connected in the molecule or in the polymeric repeating unit. Bicerano's method uses Fedor's (35) and van Krevelen's (123,163) group contribution values. Both references provide solubility parameter predictions of a number of polymers.

TABLE 1. SELECTED SOLVENTS FOR USE IN POLYMER SOLVENCY TESTING

Solvent	$\delta$ (MPa <sup>1/2</sup> )
POORLY HYDROGEN BONDED	
<i>n</i> -Pentane	14.3
<i>n</i> -Heptane	15.1
Methylcyclohexane	16.0
Solvesso 150	17.4
Toluene	18.2
Tetrahydronaphthalene	19.4
<i>o</i> -Dichlorobenzene	20.5
1-Bromonaphthalene	21.7
Nitroethane	22.7
Acetonitrile	24.1
Nitromethane	26.0
MODERATELY HYDROGEN BONDED	
Diethyl ether	15.2
Diisobutyl ketone	16.0
<i>n</i> -Butyl acetate	17.4
Methyl propionate	18.2
Dibutyl phthalate	19.0
Dioxane	20.3
Dimethyl phthalate	21.9
2,3-Butylene carbonate	24.8
Propylene carbonate	27.2
Ethylene carbonate	30.1
STRONGLY HYDROGEN BONDED	
2-Ethyl hexanol	19.4
Methyl isobutyl carbinol	20.5
2-Ethyl butanol	21.5
<i>n</i> -Pentanol	22.3
<i>n</i> -Butanol	23.3
<i>n</i> -Propanol	24.3
Ethanol	26.0
Methanol	29.7

TABLE 2. GROUP CONTRIBUTIONS TO COHESIVE ENERGY DENSITY

Group	F [MPa <sup>1/2</sup> cm <sup>3</sup> /mol]		$\Delta E_i^v$ (J/mol)	
	Small (112)	van Krevelen (121)	Hoy (61)	van Krevelen and Hoftyzer (163)
<b>2.1. CARBON-CONTAINING GROUPS</b>				
-CH <sub>3</sub>	437	420	303	9630
\CH <sub>2</sub>	272	280	269	4190
\CH-	57	140	176	420
\C\	-190	0	65	-5580
=CH <sub>2</sub>	388	-	259	-
=CH-	277	222	249	-
=C\	39	82	173	-
-CH=(aromatic)	-	-	240	-
-C=(aromatic)	-	-	201	-
-CH(CH <sub>3</sub> )-	495	560	(479)	(10060)
-C(CH <sub>3</sub> ) <sub>2</sub> -	685	841	(672)	(13700)
-CH=CH-	454	444	497	10200
-C=C-	265	304	421	4860
CH <sub>3</sub> \H C=C\	(704)	724	(725)	(14500)
H-C≡C-	583	-	-	-
-C≡C-	454	-	-	-
Cyclopentyl	-	1380	1300	-
Cyclohexyl	-	1660	1470	-
Phenyl	1500	1520	(1400)	31000
p-Phenylenes	1350	1380	(1440)	25140
Naphthyl	2340	-	-	-
<b>2.2. OXYGEN-CONTAINING GROUPS</b>				
-O-, ether	143	255	235	6290
-O-, epoxide	-	-	360	-
-OH	-	754	462	-
-OH, aromatic	-	-	350	-
-(C=O)-	562	685	538	-
-(C=O)-O-	634	511	688	13410
-(C=O)-OH	-	651	(998)	-
-O-(C=O)-O-	-	767	(904)	-
-(C=O)-O-(C=O)-	-	767	1160	-
<b>2.3. NITROGEN-CONTAINING GROUPS</b>				
-NH <sub>2</sub>	-	-	464	-
-NH-	-	-	368	-
-N\	-	-	125	-
-CH-CN	(896)	1120	(901)	25420
-CN	839	982	725	25000
-(C=O)-NH-	-	1290	(906)	60760
-O-(C=O)-NH	-	1480	(1040)	-
-N=C=O	-	-	734	-
<b>2.4. OTHER GROUPS</b>				
-H	164-205	140	-103 (acidic dimer)	-
-S-	460	460	428	8800
-SH	644	-	-	-
-F	(250)	164	84	4470
-Cl (primary)	552	471	420	12990
-Br (primary)	695	614	528	15500
-I	870	-	-	-
-CF <sub>2</sub> -	307	-	-	-
-CF <sub>3</sub>	561	-	-	-
-O-N=O	900	-	-	-
-NO <sub>2</sub>	900	-	-	-
-PO <sub>4</sub>	1020	-	-	-
-Si-	-77	-	-	-

TABLE 2. cont'd

Group	F [MPa <sup>1/2</sup> cm <sup>3</sup> /mol]		$\Delta E_i^v$ (J/mol)	
	Small (112)	van Krevelen (121)	Hoy (61)	van Krevelen and Hoftyzer (163)
<b>2.5. STRUCTURAL FEATURES</b>				
Conjugation	41-61	-	-	48
cis	-	-	-	-15
trans	-	-	-	-28
Ring, 4 member	-	-	-	159
5 member	215-235	-	-	-
6 member	194-215	-	-	-
Subscription, ortho	-	-	-	-48
meta	-	-	-	20
				14

TABLE 3. CONTRIBUTIONS TO  $E_{coh}$  AND  $V^a$ 

Group	$E_{coh}$ (J/mol)	$V$ (cm <sup>3</sup> /mol)
-CH <sub>3</sub>	4710	33.5
\CH <sub>2</sub>	4940	16.1
\CH-	3430	-1.0
\C\	1470	-19.2
=CH <sub>2</sub>	4310	28.5
=CH-	4310	13.5
=C\	4310	-5.5
H-C≡	3850	27.4
-C≡	7070	6.5
Phenyl	31940	71.4
Phenylene: o, m, p	31940	52.4
Phenyl (trisubstituted)	31940	33.4
(tetrasubstituted)	31940	14.4
(pentasubstituted)	31940	-4.6
(hexasubstituted)	31940	-23.6
Ring closure, 5+ atoms	1050	16.0
3 or 4 atoms	3140	18.0
Conjugation in ring for each double bond	1670	-2.2
Halogen attached to carbon atom	-20% of $E_{coh}$ of halogen	4.0
-F	4190	18.0
-F, disubstituted	3560	20.0
trisubstituted	2300	22.0
-CF <sub>2</sub> -, perfluoro compounds	4270	23.0
-CF <sub>3</sub> , perfluoro compounds	4270	57.5
-Cl, disubstituted	11550	24.0
trisubstituted	9630	26.0
-Br, disubstituted	7530	27.3
trisubstituted	15490	30.0
-Br, disubstituted	12350	31.0
trisubstituted	10670	32.4
-I, disubstituted	19050	31.5
trisubstituted	16740	33.5
-CN	16330	37.0
-OH	25530	24.0
-O, disubstituted or adjacent C atoms	29800	10.0
-O-	21850	13.0
-CHO, aldehyde	3350	3.8
-CO-	21350	22.3
-COOH	17370	10.8
-COO-	27630	28.5
-CO <sub>3</sub> <sup>2-</sup> , carbonate	18000	18.0
-CO <sub>3</sub> <sup>2-</sup> , anhydride	17580	22.0
	30560	30.0

TABLE 3. cont'd

Group	$E_{coh}$ (J/mol)	$V$ (cm <sup>3</sup> /mol)
HCOO-, formate	18000	32.5
-CO <sub>2</sub> CO <sub>2</sub> -, oxalate	26790	37.3
-HCO <sub>3</sub> <sup>-</sup>	12560	18.0
-COF	13400	29.0
-COCl	17580	38.1
-COBr	24150	41.6
-COI	29300	48.7
-NH <sub>2</sub>	12560	19.2
-NH-	8370	4.5
-N\	4190	-9.0
-N=	11720	5.0
-NNHH <sub>2</sub>	21980	-
-N(NH <sub>2</sub> )-	16740	16.0
H	16740	16.0
-N=C=N-	20090	-
-N≡C	11470	-
-NF <sub>2</sub>	18840	23.1
-NF-	7660	33.1
-CONH <sub>2</sub>	5070	24.5
-CONH-	41860	17.5
-CON-	33490	9.5
-C(=O)N	29510	-7.7
-C(=O)O	27630	11.3
-C(=O)N	43950	27.0
-NHCOO-	26370	18.5
-NHCONH-	50230	-
O	41860	-
-N=C-N-	20930	-14.5
-N=C-N-	37000	-
-NCO	28460	35.0
-ONH <sub>2</sub>	19050	20.0

TABLE 3. cont'd

Group	$E_{coh}$ (J/mol)	$V$ (cm <sup>3</sup> /mol)
$\text{C}=\text{N}-\text{OH}$	25120	11.3
$-\text{CH}=\text{NOH}$	25120	24.0
$-\text{NO}_2$ , aliphatic	29300	24.0
$-\text{NO}_2$ , aromatic	15360	32.0
$-\text{NO}_3$	20930	33.5
$-\text{NO}_2$ , nitrate	11720	33.5
$-\text{NHNO}_2$	39770	28.7
$-\text{NNO}-$	27210	10.0
$-\text{SH}$	14440	28.0
$-\text{S}-$	14150	12.0
$-\text{S}_2-$	23860	23.0
$-\text{S}_3-$	13400	47.2
$\text{S}=\text{O}$	39140	-
$\text{SO}_3$	18840	27.6
$\text{SO}_4$	28460	31.6
$-\text{SO}_2\text{Cl}$	37070	43.5
$-\text{SCN}$	20090	37.0
$-\text{NCS}$	25120	40.0
P	9420	-1.0
$\text{PO}_3$	14230	22.7
$\text{PO}_4$	20930	28.0
$\text{PO}_3-\text{OH}$	31810	32.2
Si	3390	0
$\text{SiO}_4$	21770	20.0
B	13810	-2.0
$\text{BO}_3$	0	20.4
Al	13810	-2.0
Ga	13810	-2.0
In	13810	-2.0
Tl	13810	-2.0
Ge	8080	-1.5
Sn	11300	1.5
Pb	17160	2.5
As	12980	7.0
Sb	16330	8.9
Bi	21350	9.5
Se	17160	16.0
Te	20090	17.4
Zn	14480	2.5
Cd	17790	6.5
Hg	22810	7.5

<sup>a</sup> Ref. 163.TABLE 4. SOLUBILITY PARAMETER I: COMPONENT GROUP CONTRIBUTIONS<sup>a</sup>

Structural Group	$F_{di}$ (J <sup>1/2</sup> cm <sup>3/2</sup> /mol)	$F_{pi}$ (J <sup>1/2</sup> cm <sup>3/2</sup> /mol)	$E_{hi}$ (J/mol)
$-\text{CH}_3$	420	0	0
$\text{CH}_2$	270	0	0
$\text{CH}-$	80	0	0
$\text{C}\backslash$	-70	0	0
$=\text{CH}_2$	400	0	0
$=\text{CH}-$	200	0	0
$=\text{C}\backslash$	70	0	0
	1620	0	0
	1430	110	0
	1270	110	0
-F	(220)	-	-
-Cl	450	550	400
-Br	(550)	-	-
-CN	430	1100	2500
-OH	210	500	20000
-O-	100	400	3000
-COH	470	800	4500
-CO-	290	770	2000
-COOH	530	420	10000
-COO-	390	490	700
HCOO-	530	-	-
-NH <sub>2</sub>	280	-	8400
-NH-	160	210	3100
-N\	20	800	5000
-NO <sub>2</sub>	500	1070	1500
-S-	440	-	-
=PO <sub>4</sub> -	740	1890	13000
Ring	190	-	-
One plane of symmetry	-	0.50 ×	-
Two planes of symmetry	-	0.25 ×	-
More planes of symmetry	-	0 ×	0 ×

<sup>a</sup> Ref. 163.TABLE 5. SOLUBILITY PARAMETER II: COMPONENT GROUP CONTRIBUTIONS<sup>a</sup>

Group	$F_{ti}$ (J cm <sup>3</sup> ) <sup>1/2</sup> /mol)	$F_{pi}$ (J cm <sup>3</sup> ) <sup>1/2</sup> /mol)	$V_i$ (cm <sup>3</sup> /mol)	$\Delta_{Ti}^*$	$\Delta_{Ti}^{(P)}$
$-\text{CH}_3$	303.5	0	21.55	0.023	0.022
$\text{CH}_2$	269.0	0	15.55	0.020	0.020
$\text{CH}-$	176.0	0	9.56	0.012	0.013
$\text{C}\backslash$	65.5	0	3.56	0	0.04
$=\text{CH}_2$	259	67	19.17	0.018	0.019
$=\text{CH}-$	249	59.5	13.18	0.018	0.0185
$=\text{C}\backslash$	173	63	7.18	0	0.013
$\text{CH}_{\text{aromatic}}$	241	62.5	13.42	0.011	0.018
$\text{C}_{\text{aromatic}}$	201	65	7.42	0.011	0.015
$-\text{HC}=\text{O}$	600	532	23.3	0.048	0.045

TABLE 5. cont'd

Group	$F_{ti}$ (J cm <sup>3</sup> ) <sup>1/2</sup> /mol)	$F_{pi}$ (J cm <sup>3</sup> ) <sup>1/2</sup> /mol)	$V_i$ (cm <sup>3</sup> /mol)	$\Delta_{Ti}^*$	$\Delta_{Ti}^{(P)}$
-CO-	538	525	17.3	0.040	0.040
-COOH	565	415	26.1	0.039	0.039
-COO-	640	528	23.7	0.047	0.050
-CO-O-CO-	1160	1160	41.0	0.086	0.086
-CN	725	725	8.2	0.054	0.054
-N=C=O	736	725	35.8	0.062	0.055
-N(HCO)-	1020	900	34.3	0.071	0.084
-CONH <sub>2</sub>	1200	895	28.3	0.054	0.073
-CONH-	1131	890	34.8	0.078	0.094
-OCONH-	1265	485	10.65	0.082	0.034
-OH-H-bonded	485	485	12.45	0.082	0.049
-OH, primary	675	675	12.45	0.082	0.049
secondary	591	591	12.45	0.082	0.049
tertiary	(500)	(500)	12.45	0.082	0.049
phenolic	350	350	12.45	0.031	0.006
-O-, ether	235	216	6.45	0.021	0.018
acetal	236	102	19.5	0.018	0.018
epoxide	361	156	6.45	0.027	0.027
-NH <sub>2</sub>	464	464	17.0	0.031	0.035
-NH-	368	368	11.0	0.031	0.025
-N\	125	125	12.6	0.014	0.009
-S-	428	428	18.0	0.015	0.032
-F	845	73.5	11.2	0.018	0.006
-Cl, primary	419.5	307	19.5	0.017	0.031
secondary	426	315	19.5	0.017	0.032
aromatic	330	81.5	19.5	0.017	0.025
Cl	705	572	39.0	0.034	0.052
Cl	528	123	25.3	0.010	0.039
Br, aliphatic	422	100	25.3	0.010	0.031
Base value, B	277	-	-	0	0.012
Ring, non-aromatic	159	203	-	0	0.003
4-member	43	85	-	0	-0.0035
5-member	-48	61	-	0	-0.007
6-member	92	0	-	0	0.0035
7-member	47.5	-19.8	-	0	-0.001
Conjugation, isomerism	-14.6	-14.6	-	0	-0.002
cis	-27.6	-27.6	-	0	-0.0015
trans	20.2	-13.3	-	0	0.001
Aromatic substitution, ortho	13.5	-24.3	-	0	0.006
meta	83	-34.0	-	0	0.006

<sup>a</sup> Ref. (178-179).TABLE 6. EQUATIONS TO BE USED FOR HOY'S SYSTEM<sup>a</sup>

Formulae	Solvents	Amorphous polymers
Additive molar functions	$F_t = \sum n_i F_{t,i}$ $F_p$	

TABLE 6. cont'd

Formulae	Solvents	Amorphous polymers
	$\delta_p = \delta_t \left( \frac{1}{\alpha} \frac{F_p}{F_t + B} \right)^{1/2}$	$\delta_p = \delta_t \left( \frac{1}{\alpha^{(P)}} \frac{F_p}{F_t + B/\bar{n}} \right)^{1/2}$
	$\delta_h = \delta_t \left( \frac{\alpha - 1}{\alpha} \right)^{1/2}$	$\delta_h = \delta_t \left( \frac{\alpha^{(P)} - 1}{\alpha^{(P)}} \right)^{1/2}$
	$\delta_d = (\delta_t^2 - \delta_p^2 - \delta_h^2)^{1/2}$	$\delta_d = (\delta_t^2 - \delta_p^2 - \delta_h^2)^{1/2}$

<sup>a</sup> In the equations given here,  $F_t$  is always combined with a Base value,  $\alpha$  is the molecular aggregation number, and  $\bar{n}$  the number of repeating units per polymer chain segment.

## D. SOLUBILITY PARAMETER TABLES

TABLE 7. SOLUBILITY PARAMETERS OF SOLVENTS IN ALPHABETICAL ORDER

Solvent	CAS number	Solubility parameter $\delta$		H-bonding group
		(MPa <sup>1/2</sup> )	(cal/cm) <sup>1/2</sup>	
Acetaldehyde	75-07-0	21.1	10.3	m
Acetic acid	64-19-7	20.7	10.2	s
Acetic anhydride	108-24-7	21.1	10.3	s
Acetone	67-64-1	20.3	9.9	m
Acetonitrile	75-07-8	24.3	11.9	p
Acetophenone	98-86-2	21.7	10.6	m
Acetyl chloride	75-36-5	19.4	9.5	m
Acetylmorpholine (N)	1696-20-4	23.7	11.6	m
Acetylpiridine (N)	618-42-8	22.9	11.2	s
Acetylpyrrolidine (N)	1072-83-9	23.3	11.4	s
Acrolein	107-02-8	20.1	9.8	s
Acrylic acid	79-10-7	24.6	12.0	s
Acrylonitrile	107-13-1	21.5	10.5	p
Allyl acetate	591-87-7	18.8	9.2	m
Allyl alcohol	107-18-6	24.1	11.8	s
Allyl chloride	107-05-1	18.0	8.8	m
Ammonia	7664-41-7	33.4	16.3	s
Amyl acetate (iso)	625-16-1	16.0	7.8	m
(normal)	628-63-7	17.4	8.5	m
(secondary)	626-38-0	17.0	8.3	m
Amyl alcohol	75-85-4	20.5	10.0	s
Amyl alcohol (normal)	71-41-0	22.3	10.9	s
Amylamine (normal)	110-58-7	17.8	8.7	s
Amyl bromide (1-bromopentane)	110-53-2	15.6	7.6	m
Amyl chloride (1-chloropentane)	543-59-9	17.0	8.3	m
Amylene (2-methyl-2-butene)	513-35-9	14.1	6.9	p
Amyl ether (pentyl ether)	693-65-2	14.9	7.3	m
Amyl formate (iso)	110-45-2	16.4	8.0	m
(normal)	638-49-3	17.2	8.5	m
Amyl iodide (1-iodopentane)	628-17-1	17.2	8.4	m
Anethole (para)	4180-23-8	17.2	8.4	m
Aniline	65-53-3	21.1	10.3	s
Anthracene	120-12-7	20.3	9.9	p
Apco #18 solvent		15.3	7.5	p
Apco #140 solvent		14.9	7.3	p
Apco thinner		16.0	7.8	p
Aroclor 1248	12672-29-6	18.0	8.8	m
Benzaldehyde	100-52-7	19.2	9.4	p
Benzene	71-43-2	18.8	9.2	p
Benzonitrile	100-47-0	17.2	8.4	s
Benzyl alcohol	100-51-6	24.8	12.1	p
Bicyclohexyl	92-51-3	17.4	8.5	p
Bromobenzene	108-86-1	20.3	9.9	p
1-Bromonaphthalene	90-11-9	21.7	10.6	p
Bromostyrene (ortho)	2039-88-5	20.1	9.8	p
1,3-Butadiene	106-99-0	14.5	7.1	

TABLE 7. cont'd

Solvent	CAS number	Solubility parameter $\delta$ (MPa <sup>1/2</sup> )	Solubility parameter $\delta$ (cal/cm) <sup>1/2</sup>	H-bonding group
n-Butane	106-97-8	13.9	6.8	p
1,3-Butanediol	107-88-0	23.7	11.6	s
1,4-Butanediol	110-63-4	24.8	12.1	s
2,3-Butanediol	513-85-9	22.7	11.1	s
Butyl acetate (iso)	540-88-5	17.0	8.3	m
Butyl acetate	123-86-4	17.4	8.5	m
n-Butyl acetate	105-46-4	16.8	8.2	m
sec-Butyl acetate	1663-39-4	17.4	8.5	m
Butyl acrylate (iso)	141-32-2	18.0	8.8	m
n-Butyl acrylate	78-83-1	21.5	10.5	s
Butyl alcohol (iso) (2-methyl-1-propanol)	71-36-3	23.3	11.4	s
n-Butyl alcohol (1-butanol)	15892-23-6	22.1	10.8	s
sec-Butyl alcohol (2-butanol)	75-65-0	21.7	10.6	s
tert-Butyl alcohol (2-methyl-2-propanol)	109-73-9	17.8	8.7	s
n-Butylamine	109-65-9	17.8	8.7	m
n-Butyl bromide (1-bromobutane)	78-76-2	17.2	8.4	m
sec-Butyl bromide (2-bromobutane)	539-90-2	16.0	7.8	m
Butyl (iso) butyrate (normal)	109-21-7	16.6	8.1	m
Butyl (normal) butyrate (normal)	507-20-0	16.6	8.1	m
Butyl chloride (iso) (2-chloro-2-methylpropane)	4437-85-9	24.8	12.1	m
Butylene-2,3 carbonate	115-11-7	13.7	6.7	p
Butylene (iso) (2-methylpropene)	142-96-1	16.0	7.8	m
Butyl ether	762-75-4	16.8	8.2	m
Butyl formate (iso)	592-84-7	18.2	8.9	m
(normal)	542-69-8	17.6	8.6	m
Butyl iodide (normal) (1-iodobutane)	138-22-7	19.2	9.4	m
Butyl lactate (normal)	97-88-1	16.8	8.2	m
Butyl methacrylate	590-01-2	18.0	8.8	m
Butyl propionate	123-95-5	15.3	7.5	m
Butyl stearate	123-72-8	18.4	9.0	m
Butyraldehyde	79-31-2	21.1	10.3	s
Butyric acid (iso) (2-methylpropionic acid)	107-92-6	21.5	10.5	s
Butyric (normal)	96-48-0	25.8	12.6	m
Butyrolactone, $\gamma$	78-82-0	20.1	9.8	p
Butyronitrile (iso)	109-74-0	21.5	10.5	p
(normal)	105-60-2	26.0	12.7	m
Caprolactam, $\varepsilon$	502-44-3	20.7	10.1	m
Capronitrile (heptyl cyanide)	124-12-9	19.2	9.4	p
Carbon disulfide	75-15-0	20.5	10.0	p
Carbon tetrachloride	56-23-5	17.6	8.6	p
Celanese solvent 601		18.8	9.2	m
Chloroacetonitrile	920-37-6	25.8	12.6	p
Chlorobenzene	108-90-7	19.4	9.5	p
Chloroethyl acetate ( $\beta$ )	542-58-5	19.8	9.7	m
Chloroform	67-66-3	19.0	9.3	p
Chlorostyrene (ortho or para)	2039-87-4	19.4	9.5	p
Chlorotoluene (para)	106-43-4	18.0	8.8	p
Cresol (meta)	108-39-4	20.9	10.2	s
Cyclobutanedione	14406-53-3	22.5	11.0	m
Cyclohexane	110-82-7	16.8	8.2	p
Cyclohexanol	108-93-0	23.3	11.4	s
Cyclohexanone	108-94-1	20.3	9.9	m
Cyclopentane	287-92-3	17.8	8.7	p
Cyclopentanone	120-92-3	21.3	10.4	m
Cymene (para) (2-isopropyl toluene)	99-87-6	16.8	8.2	p
Decahydronaphthalene (cis and trans) (Decalin)	91-17-8	18.0	8.8	p
Decane (normal)	124-18-5	13.5	6.6	p
Decyl acrylate (iso)	2156-96-9	16.8	8.2	m
Diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)	123-42-2	18.8	9.2	m
Diacetone alcohol methyl ether (Pentoxone)	107-70-0	16.8	8.2	m
Diametylphthalazine (N,N)	18940-57-3	28.0	13.7	m
Dibenzyl ether	131-18-0	18.6	9.1	m
Dibenzyl phthalate	103-50-4	19.2	9.4	m

TABLE 7. cont'd

Solvent	CAS number	Solubility parameter $\delta$			H-bonding group
		(MPa $^{1/2}$ )	(cal/cm) $^{1/2}$		
Dibromoethane-1,2	106-93-4	21.3	10.4		p
Dibromoethylene-1,2 ( <i>cis</i> and <i>trans</i> )	540-49-8	20.7	10.1		p
Dibutoxyethyl phthalate (Kronisol)	117-83-9	16.4	8.0		m
Dibutylamine	111-92-2	16.6	8.1		s
Dibutyl fumarate	105-75-9	18.4	9.0		m
Dibutyl maleate	105-76-0	18.4	9.0		m
Dibutyl phenyl phosphate	2528-36-1	17.8	8.7		m
Dibutyl phthalate	84-74-2	19.0	9.3		p
Dibutyl sebacate	109-43-3	18.0	9.2		m
Dichloroacetic acid	79-43-6	22.5	11.0		s
Dichlorobenzene ( <i>ortho</i> )	95-50-1	20.5	10.0		p
Dichlorodifluoromethane (Freon 12)	75-71-8	11.3	5.5		p
Dichloroethyl ether	623-46-1	20.1	9.8		m
Dichloroethylene, <i>cis</i> -1,2	156-59-2	18.6	9.1		p
trans-1,2	156-60-5	18.4	9.0		p
Dichlorofluoromethane (Freon 21)	75-43-4	17.0	8.3		p
Dichloropropene-1,2	78-87-5	18.4	9.0		p
Dichloropropene-2,2	594-20-7	16.8	8.2		p
Diethylacetamide ( <i>N,N</i> )	685-91-6	20.3	9.9		p
Diethylamine	109-89-7	16.4	8.0		m
Diethyl carbonate	105-58-8	18.0	8.8		s
Diethylene glycol	111-46-6	24.8	12.1		m
Diethylene glycol monobutyl ether (normal)	112-34-5	19.4	9.5		m
Diethylene glycol monobutyl ether	112-34-5	20.9	10.2		m
Diethylene glycol monobutyl ether acetate	124-17-4	17.4	8.5		m
Diethylene glycol monolaurate	141-20-8	17.8	8.7		m
Diethyl ether	60-29-7	15.1	7.4		m
Diethylformamide ( <i>N,N</i> )	617-84-5	21.7	10.6		m
Diethyl ketone	96-22-0	18.0	8.8		m
Diethyl maleate	141-05-9	20.3	9.9		m
Diethyl oxalate	95-92-1	17.6	8.6		m
Diethyl phthalate	84-66-2	20.5	10.0		m
Diethyl-2,2-propanediol-1,2 (heptylene glycol)	115-76-4	20.3	9.9		s
Diethyl sulfone	597-35-3	25.4	12.4		m
Difluorotetrachloroethane (Freon 112)	76-11-9	16.0	7.8		p
Diformylpiperazine ( <i>N,N</i> )	4164-39-0	31.5	15.4		m
Dihexyl ether	112-58-3	16.4	8.0		m
Di-n-hexyl phthalate	108-83-8	18.2	8.9		m
Diisobutylene	107-39-1	15.8	7.7		p
Diisobutyl ketone	108-83-8	16.0	7.8		m
Diisodecyl phthalate	26761-40-0	14.7	7.2		m
Diisopropyl ether	108-20-3	14.1	6.9		m
Diisopropyl ketone	565-80-0	16.4	8.0		m
Dimethylacetamide ( <i>N,N</i> )	127-19-5	22.1	10.8		m
Dimethylaniline	121-69-7	19.8	9.7		m
Dimethyl-2,2-butanediol-1,2 (isobutylene glycol)	558-43-0	22.9	11.2		s
Dimethyl-2,2-butanediol-1,3	76-09-3	20.5	10.0		s
Dimethyl carbonate	616-38-6	20.3	9.9		m
Dimethyl ether	115-10-6	18.0	8.8		m
Dimethylformamide ( <i>N,N</i> )	68-12-2	24.8	12.1		m
Dimethyl malonate	108-59-8	22.5	11.0		m
Dimethylnitroamine ( <i>N,N</i> )	62-75-9	26.8	13.1		m
Dimethyl oxalate	553-90-2	22.5	11.0		m
Dimethyl phosphite	868-85-9	25.6	12.5		m
Dimethyl phthalate	131-11-3	21.9	10.7		m
Dimethyl siloxane	9016-00-6	10.0-12.1	4.9-5.9		p
Dimethyl sulfide	75-18-3	19.2	9.4		p
Dimethyl sulfoxide	67-68-5	29.7	14.5		m
Dimethyltetramethylene sulfone	1003-78-7	24.6	12.0		m
Diocetyl adipate	103-23-1	17.8	8.7		m
Diocetyl phthalate	117-81-7	24.8	12.1		m
Diocetyl sebacate	1222-62-3	17.8	8.7		m
Dioxane-1,4	123-91-1	16.2	7.9		m

TABLE 7. cont'd

Solvent	CAS number	Solubility parameter $\delta$			H-bonding group
		(MPa $^{1/2}$ )	(cal/cm) $^{1/2}$		
Dioxolane-1,3	646-06-0	17.6	8.6		m
Dipentene	138-86-3	20.5	10.0		m
Diphenyl ether	101-84-8	20.9	10.2		m
Diphenyl 2-ethylhexyl phosphate	1241-94-7	17.4	8.5		p
Dipropylene glycol	110-98-5	20.7	10.1		m
Dipropylene glycol monomethyl ether	34590-94-8	17.6	8.6		m
Dipropyl phthalate	131-16-8	20.5	10.0		s
Dipropyl sulfone	598-03-8	23.1	11.3		m
Dodecane	112-40-3	16.2	7.9		p
Dodecanol-1	112-53-8	20-21	9.8		s
Epichlorohydrin	106-89-8	22.5	11.0		s
Ethane	74-84-0	12.3	6.0		p
Ethylacetamide ( <i>N</i> )	625-50-3	25.2	12.3		s
Ethyl acetate	141-78-6	18.6	9.1		m
Ethyl acrylate	140-88-5	17.6	8.6		m
Ethyl alcohol	64-17-5	26.0	12.7		s
Ethylamine	75-04-7	20.5	10.0		s
Ethyl amyl ketone (3-octanone)	106-68-3	16.8	8.2		p
Ethylbenzene	100-41-4	18.0	8.8		m
Ethyl benzoate	93-89-0	16.8	8.2		m
Ethyl bromide (bromoethane)	74-96-4	19.6	9.6		m
Ethyl-2-butanol-1	97-95-0	21.5	10.5		s
Ethyl n-butyrate	105-54-4	17.4	8.5		m
Ethyl caprylate	106-32-1	14.9	7.3		m
Ethyl chloride	75-00-3	18.8	9.2		m
Ethyl cyanoacetate	105-56-6	22.5	11.0		m
Ethylene bromide	593-60-2	19.8	9.7		p
Ethylene carbonate	96-49-1	30.1	14.7		m
Ethylene chlorohydrin (2-chloroethanol)	107-07-3	25.0	12.2		s
Ethylene cyanohydrin (3-hydroxypropionitrile)	109-78-4	31.1	15.2		s
Ethylenediamine	107-15-3	25.2	12.3		s
Ethylene dichloride (1,2-dichloroethane)	107-06-2	20.1	9.8		p
Ethylene glycol	107-21-1	29.9	14.6		s
Ethylene glycol diacetate	111-55-7	20.5	10.0		m
Ethylene glycol diethyl ether	629-14-1	17.0	8.3		m
Ethylene glycol dimethyl ether	110-71-4	17.6	8.6		m
Ethylene glycol methyl ether acetate	110-49-6	18.8	9.2		m
Ethylene glycol monobenzyl ether	622-08-2	22.3	10.9		m
Ethylene glycol monobutyl ether	111-76-2	19.4	9.5		m
Ethylene glycol monoethyl ether (2-ethoxyethanol; Cellusolve)	110-80-5	21.5	10.5		m
Ethylene glycol monomethyl ether (2-methoxyethanol)	109-86-4	23.3	11.4		m
Ethylene glycol monophenyl ether	122-99-6	23.5	11.5		m
Ethylene oxide	75-21-8	22.7	11.1		m
Ethylene formamide ( <i>N</i> )		28.4	13.9		s
Ethyl formate	109-94-4	19.2	9.4		m
Ethyl-2-hexanediol-1,3 (octylene glycol)	94-96-2	19.2	9.4		s
Ethylhexanol	104-76-7	19.4	9.5		s
Ethyl hexyl acrylate	103-11-7	16.0	7.8		m
Ethylidene chloride	75-34-3	18.2	8.9		p
Ethyl iodide (iodoethane)	75-03-6	19.2	9.4		m
Ethyl isobutyl ether	627-02-1	15.3	7.5		m
Ethyl isobutyrate	97-62-1	16.2	7.9		m
Ethyl lactate	687-47-8	20.5	10.0		m
Ethyl mercaptan (ethane thiol)	75-08-1	18.8	9.2		p
Ethyl methacrylate	97-63-2	17.0	8.3		m
Ethyl morpholine ( <i>N</i> )	100-74-3	18.2	8.9		s
Ethyl orthoformate (triethyl orthoformate)	122-51-0	17.0			

TABLE 7. cont'd

Solvent	Solubility parameter $\delta$			H-Bonding Group	Solubility parameter $\delta$			H-bonding group
	CAS number	MPa <sup>1/2</sup>	(cal/cm) <sup>1/2</sup>		CAS number	(MPa) <sup>1/2</sup>	(cal/cm) <sup>1/2</sup>	
Formylmorpholine ( <i>N</i> )	4394-85-8	26.6	13.0	m	107-41-5	19.8	9.7	s
Formylpiperidine ( <i>N</i> )	2591-86-8	23.5	11.5	m		17.4	8.5	m
Furan	110-00-9	19.2	9.4	m	554-12-1	18.2	8.9	m
Furfural (2-furaldehyde)	98-01-1	22.9	11.2	m	107-87-9	17.8	8.7	m
Furfuryl alcohol	98-00-0	25.6	12.5	m	1977-37-3	25.6	12.5	m
Glycerol	56-81-5	33.8	16.5	s	872-50-4	23.1	11.3	m
Heptane (normal)	142-82-5	15.1	7.4	s	119-36-8	21.7	10.6	m
Heptyl alcohol (normal)	111-70-6	21.7	10.6	p	98-83-9	17.4	8.5	p
Hexamethylphosphoramide	680-31-9	21.5	10.5	s	Methyl styrene ( $\alpha$ )	26.4	12.9	m
Hexane (normal)	110-54-3	14.9	7.3	s	Methyltetramethylene sulfone	624-24-8	16.2	m
Hexanediol-2,5	2935-44-6	21.2	10.3	p	Methyl <i>n</i> -valerate	110-91-8	22.1	s
Hexene-1	592-41-6	15.1	7.4	p	Morpholine	91-20-3	20.3	p
Hexyl alcohol (normal)	111-27-3	21.9	10.7	s	Naphthalene	463-82-1	12.9	s
Hydrazine	302-10-2	37.3	18.1	s	Neopentane	126-30-7	22.5	s
Hydrogen	1333-74-0	6.9	3.0	p	Neopentyl glycol	98-95-3	20.5	p
Hydrogenated terphenyl (Monsanto HB-40)		18.4	9.0	p	Nitrobenzene	79-24-3	22.7	p
Hydrogen cyanide	74-90-8	24.8	12.1	s	Nitroethane	75-52-5	26.0	p
Iodobenzene	591-50-4	20.7	10.1	p	Nitromethane		14.3	p
Isophorone	78-59-1	18.6	9.1	m	Nitro- <i>n</i> -octane	108-03-2	21.1	p
Isoprene	78-79-5	15.1	7.4	p	Nitro-1-propane	79-46-9	20.3	p
Lauryl alcohol	112-53-8	16.6	8.1	s	Nitro-2-propane	25154-52-3	19.2	s
Low odor mineral spirits		14.1	6.9	p	Nonyl phenol	Octane (normal)	15.6	p
Maleic anhydride	108-31-6	27.8	13.6	s	Octyl alcohol (normal)	111-65-9	7.6	p
Malononitrile	109-77-3	30.9	15.1	p	Pentachloroethane	76-01-7	19.2	p
Mesitylene	108-67-8	18.0	8.8	p	Pentane (normal)	109-66-0	14.3	s
Mesityl oxide	141-79-7	18.4	9.0	m	Pentanediol-1,5	111-29-5	23.5	s
Methacrylic acid	79-41-4	22.9	11.2	s	Pentanediol-2,4	625-69-4	22.1	s
Methane	74-82-8	11.0	5.4	p	Perchloroethylene	127-18-4	19.0	p
Methanol	67-56-1	29.7	14.5	s	Perfluoroheptane	335-57-9	11.9	p
Methoxy-4-methyl-4-pentanol-2		17.4	8.5	s	Perfluoromethylcyclohexane	355-02-2	12.3	p
Methoxy-4-methyl-4-pentanone-2	107-70-0	17.0	8.3	m	Phenanthrene	85-01-8	20.1	s
Methylacetamide	79-16-3	29.9	14.6	m	Phenylhydrazine	100-63-0	25.6	s
Methyl acetate	79-20-9	19.6	9.6	m	Pine oil		17.6	p
Methyl acrylate	96-33-3	18.2	8.9	m	Piperidine	110-89-4	17.8	p
Methylamine	74-89-5	22.9	11.2	s	Piperidone	675-20-7	27.8	s
Methyl amyl acetate	108-84-9	16.4	8.0	m	Propane	74-98-6	13.1	p
Methyl amyl ketone	110-43-0	17.4	8.5	m	Propiolactone	57-57-8	27.2	m
Methyl benzoate	95-58-3	21.5	10.5	m	Propionic acid	79-09-4	20.3	s
Methyl bromide	74-83-9	19.6	9.6	m	Propionic anhydride	123-62-6	20.5	s
Methyl <i>n</i> -butyl ketone	591-78-6	17.0	8.3	m	Propionitrile	107-12-0	22.1	p
Methyl <i>n</i> -butyrate	623-42-7	18.2	8.9	m	Propyl acetate (iso)	108-21-4	17.2	m
Methyl caprolactone		18.2	8.9	m	Propyl acetate (normal)	109-60-4	18.0	m
Methyl chloride	74-87-3	19.8	9.7	m	Propyl alcohol (2-propanol)	67-63-0	23.5	s
Methylcyclohexane	10120-28-2	16.0	7.8	p	Propyl alcohol (1-propanol)	71-23-8	24.3	s
Methylcyclohexanone	589-92-4	19.0	9.3	m	Propylbenzene (normal)	103-65-1	17.6	p
Methylene chloride	75-09-2	19.8	9.7	p	Propyl bromide (1-bromopropane)	106-94-5	18.2	m
Methylene glycolate	61192-32-3	25.4	12.4	m	Propyl butyrate	105-66-8	17.2	m
Methylene iodide	75-11-6	24.1	11.8	p	Propyl butyrate (iso)	638-11-9	16.2	m
Methyl ethyl ketone	78-93-3	19.0	9.3	m	Propyl chloride (2-chloropropane)	75-29-6	16.6	m
Methyl ethyl sulfone	594-43-4	27.4	13.4	m	Propyl chloride (1-chloropropane)	540-54-5	17.4	s
Methylformamide ( <i>N</i> )	123-39-7	32.9	16.1	s	Propylene-1,2-carbonate	108-32-7	27.2	m
Methyl formate	107-31-3	20.9	10.2	m	Propylene glycol (1,2-propanediol)	57-55-6	25.8	s
Methyl <i>n</i> -hexyl ketone	111-13-7	17.0	8.3	m	Propylene glycol methyl ether (1,2-dimethoxypropane)	7778-85-0	20.7	m
Methyl iodide	74-88-4	20.9	10.2	m	Propylene oxide	75-56-9	18.8	m
Methyl isoamyl ketone	110-12-3	17.2	8.4	m	Propyl ether (di-, normal)	111-43-3	16.0	s
Methyl isobutyl carbinol	108-11-2	20.5	10.0	s	Propyl ether (iso)	108-20-3	14.5	m
Methyl isobutyl ketone	108-10-1	17.2	8.4	m	Propyl formate	110-74-7	18.8	m
Methyl isobutyrate	547-63-7	17.0	8.3	m	Propyl propionate	106-36-5	17.4	s
Methyl isopropyl ketone	563-80-4	17.4	8.5	m	Pyridine	110-86-1	21.9	m
Methyl isovalerate	624-24-8	16.2	7.9	m	Pyrone ( $\gamma$ )	504-31-4	27.4	m
Methyl methacrylate	80-62-6	18.0	8.8	m	Pyrrolidine ( $\alpha$ ) (2-)	123-75-1	30.1	s
Methyl nonyl ketone	112-12-9	16.0	7.8	m	Quinoline	00-02-2	22.1	s
Methyl-2-pentanediol-1,3	149-31-5	21.1	10.3	s	Santicizer 8		24.3	m

TABLE 7. cont'd

TABLE 7. cont'd

Solvent	CAS number	Solubility parameter $\delta$		
		(MPa $^{1/2}$ )	(cal/cm) $^{1/2}$	H-bonding group
Shell Sol 72		14.7	7.2	p
Shell TS28 solvent		15.1	7.4	p
Silicon tetrachloride		15.1	7.4	p
Socal solvent No. 1		16.6	8.1	p
Socal solvent No. 2		16.2	7.9	p
Socal solvent No. 3		15.8	7.7	p
Solvesso 100		17.6	8.6	p
Solvesso 150		17.4	8.5	p
Styrene	100-42-5	19.0	9.3	p
Styrene oxide	96-09-3	21.5	10.5	m
Succinic anhydride	108-30-5	31.5	15.4	s
Terpene B		17.2	8.4	p
Tetrachloroethane-1,1,2,2	79-34-5	19.8	9.7	p
Tetrachloroethylene (perchloroethylene)	127-18-4	19.0	9.3	p
Tetraethylene glycol	112-60-7	20.3	9.9	s
Tetrahydrofuran	109-99-9	18.6	9.1	m
Tetrahydronaphthalene (tetralin)	119-64-2	19.4	9.5	p
Tetramethylene sulfone (sulfolane, tetrahydrothiophene 1,1-dioxide)	126-33-0	27.4	13.4	m
Tetramethyloxamide		23.3	11.4	m
Thiophene	110-02-1	20.1	9.8	m
Toluene	108-88-3	18.2	8.9	p
Tolylene diisocyanate (4-methyl-1,3-phenylene diisocyanate)	584-84-9	23.7	11.6	s
Tributylamine	102-82-9	15.8	7.7	s
Trichloroethane-1,1,2	79-00-5	19.6	9.6	p
Trichloroethylene	79-01-6	18.8	9.2	p
Trichlorofluoromethane	75-69-4	15.5	7.6	p
Trichlorotrifluoroethane (1,1,2-trichlorotrifluoroethane)	76-13-1	14.9	7.3	p
Tricresyl phosphate (tritolyphosphate)	1330-78-5	17.2	8.4	m
Triethylamine	121-44-8	15.1	7.4	s
Triethylene glycol	112-27-6	21.9	10.7	s
Triethylenetetramine	112-24-3	22.7	11.1	s
Trimethyl-3,5,5-hexanol (nonyl alcohol)	3452-97-9	17.2	8.4	s
Triphenyl phosphate	115-86-6	17.6	8.6	m
Triphenyl phosphite	101-02-0	19.0	9.3	m
Tripropylene glycol	24800-44-0	18.8	9.2	s
Tripropylene glycol methyl ether	20324-33-8	17.8	8.7	m
Turpentine	8006-64-2	16.6	8.1	p
Valeric acid (normal)	109-52-4	20.1	9.8	s
Valeronitrile (normal)	110-59-8	19.6	9.6	s
Varnolene (Varsol #2)		15.6	7.6	p
Vinyl acetate	108-05-4	18.4	9.0	m
Vinyl chloride	75-01-4	16.0	7.8	m
Vinyl toluene	622-97-9	18.6	9.1	p
V M & P naphtha		15.6	7.6	p
Water	7732-18-5	47.9	23.4	s
Xylene ( <i>p</i> -xylene)	106-42-3	18.0	8.8	p

TABLE 8. SOLUBILITY PARAMETERS OF SOLVENTS IN INCREASING ORDER OF  $\delta$ 

Solvent	$\delta$ (MPa $^{1/2}$ )
Hydrogen	6.9
Dimethyl siloxane	10.0-12.1
Methane	11.0
Dichlorodifluoromethane (Freon 12)	11.3
Fluorocarbons, aliphatic	11.3-12.7
Perfluoroheptane	11.9
Ethane	12.3
Perfluoromethylcyclohexane	12.3
Neopentane	12.9

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Propane	13.1
Decane (normal)	13.5
Butylene (iso) (2-methylpropene)	13.7
n-Butane	13.9
Amylene (2-methyl-2-butene)	14.1
Diisopropyl ether	14.1
Low odor mineral spirits	14.1
Nitro-n-octane	14.3
Pentane (normal)	14.3
1,3-Butadiene	14.5

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Propyl ether (iso)	14.5
Diisodecyl phthalate	14.7
Shell Sol 72	14.7
Amyl ether (pentyl ether)	14.9
Apco #140 solvent	14.9
Ethyl caprylate	14.9
Hexane (normal)	14.9
Trichlorotrifluoroethane (1,1,2-trichlorotrifluoroethane)	15.1
Diethyl ether	15.1
Heptane (normal)	15.1
Hexene-1	15.1
Isoprene	15.1
Shell TS28 solvent	15.1
Silicon tetrachloride	15.1
Triethylamine	15.3
Apco #18 solvent	15.3
Butyl stearate	15.3
Ethyl isobutyl ether	15.3-16.8
Fluorocarbons (aromatic)	15.5
Trichlorofluoromethane	15.6
Amyl bromide (1-bromopentane)	15.6
Octane (normal)	15.6
Varnolene (Varsol #2)	15.6
V M & P naphtha	15.6
Diisobutylene	15.8
Socal solvent No. 3	15.8
Tributylamine	15.8
Amyl acetate (iso)	16.0
Apco thinner	16.0
Butyl (iso) butyrate (normal)	16.0
Butyl ether	16.0
Diffluorotetrachloroethane (Freon 112)	16.0
Diisobutyl ketone	16.0
Ethyl hexyl acrylate	16.0
Methylcyclohexane	16.0
Methyl nonyl ketone	16.0
Propyl ether (di-, normal)	16.0
Vinyl chloride	16.0
Dioxane-1,4	16.2
Dodecane	16.2
Ethyl isobutyrate	16.2
Methyl isovalerate	16.2
Methyl <i>n</i> -valerate	16.2
Propyl butyrate (iso)	16.2
Socal solvent No. 2	16.2
Amyl formate (iso)	16.4
Dibutoxyethyl phthalate (Kronisol)	16.4
Diethylamine	16.4
Dihexyl ether	16.4
Diisopropyl ketone	16.4
Methyl amyl acetate	16.4
Butyl (normal) butyrate (normal)	16.6
Butyl chloride (iso) (2-chloro-2-methylpropane)	16.6
Diethylamine	16.6
Lauryl alcohol	16.6
Propyl chloride (2-chloropropane)	16.6
Socal solvent No. 1	16.6
Turpentine	16.6
sec-Butyl acetate	16.8
Butyl formate (iso)	16.8
Butyl methacrylate	16.8
Cyclohexane	16.8
Cymene ( <i>para</i> ) (2-isopropyl toluene)	16.8
Decyl acrylate (iso)	16.8
Diacetone alcohol methyl ether (Pentoxone)	16.8

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Dichloropropane-2,2	16.8
Ethyl amy1 ketone (3-octanone)	16.8
Ethyl benzoate	17.0
Ethyl benzoate (secondary)	17.0
Amyl chloride (1-chloropentane)	17.0
Butyl acetate (iso)	17.0
Dichlorofluoromethane (Freon 21)	17.0
Ethylene glycol diethyl ether	17.0
Ethyl methacrylate	17.0
Ethyl orthoformate (triethyl orthoformate)	17.0
Methoxy-4-methyl-4-pentanone-2	17.0
Methyl <i>n</i> -butyl ketone	17.0
Methyl <i>n</i> -hexyl ketone	17.0
Methyl isobutyrate	17.2
Amylformates (normal)	17.2
Methyl isobutyrate (normal)	17.2
Amyl iodide (1-iodopentane)	17.2
Anethole ( <i>para</i> )	17.2
Benzonitrile	17.2
sec-Butyl bromide (2-bromobutane)	17.2
Ethyl propionate	17.2
Methyl isoamyl ketone	17.2
Methyl isobutyl ketone	17.2
Propyl acetate (iso)	17.2
Propyl butyrate	17.2
Terpene B	17.2
Tricresyl phosphate (trityl phosphate)	17.2
Trimethyl-3,5,5-hexanol (nonyl alcohol)	17.2
Trimethyl-3,5,5-hexanol (normal)	17.4
Bicyclohexyl	17.4
n-Butyl acetate	17.4
Butyl acrylate (iso)	17.4
Diethylene glycol monobutyl ether acetate	17.4
Diphenyl 2-ethylhexyl phosphate	17.4
Ethyl <i>n</i> -butyrate	17.4
Methoxy-4-methyl-4-pentanol-2	17.4
Methyl amyl ketone	17.4
Methyl isopropyl ketone	17.4
Methyl-2-pentanediol monoethyl ether (Pentoxol)	17.4
Methyl styrene ( $\alpha$ )	17.4
Propyl chloride (1-chloropropane)	17.4
Propyl propionate	17.4
Solvesso 150	17.4
Butyl iodide (normal) (1-iodobutane)	17.6
Carbon tetrachloride	17.6
Diethyl oxalate	17.6
Dioxolane-1,3	17.6
Dipropylene glycol monomethyl ether	17.6
Ethyl acrylate	17.6
Ethylene glycol dimethyl ether	17.6
Pine oil	17.6
Propylbenzene (normal)	17.6
Solvesso 100	17.6
Triphenyl phosphate	17.8
Amylamine (normal)	17.8
n-Butylamine	17.8
n-Butyl bromide (1-bromobutane)	17.8
Cyclopentane	17.8
Dibutyl phenyl phosphate	17.8

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Aroclor 1248	18.0
Allyl chloride	18.0
n-Butyl acrylate	18.0
Butyl propionate	18.0
Chlorotoluene (para)	18.0
Decahydronaphthalene ( <i>cis</i> and <i>trans</i> ) (decalin)	18.0
Dibutyl sebacate	18.0
Diethyl carbonate	18.0
Diethyl ketone	18.0
Dimethyl ether	18.0
Ethylbenzene	18.0
Mesitylene	18.0
Methyl methacrylate	18.0
Propyl acetate (normal)	18.0
Xylene ( <i>p</i> -xylene)	18.0
Butyl formate (normal)	18.2
Di-n-hexyl phthalate	18.2
Ethyldiene chloride	18.2
Ethyl morpholine (normal)	18.2
Methyl acrylate	18.2
Methyl <i>n</i> -butyrate	18.2
Methyl caprolactone	18.2
Methyl propionate	18.2
Propyl bromide (1-bromopropane)	18.2
Toluene	18.2
Butyraldehyde	18.4
Dibutyl fumarate	18.4
Dibutyl maleate	18.4
Dichloroethylene <i>trans</i> -1,2	18.4
Dichloropropane-1,2	18.4
Hydrogenated terphenyl (Monsanto HB-40)	18.4
Mesityl oxide	18.4
Vinyl acetate	18.4
Diamyl phthalate	18.6
Dichloroethylene, <i>cis</i> -1,2	18.6
Ethyl acetate	18.6
Isophorone	18.6
Tetrahydrofuran	18.6
Vinyl toluene	18.6
Allyl acetate	18.8
Benzene	18.8
Celanese solvent 601	18.8
Diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)	18.8
Ethyl chloride	18.8
Ethylene glycol methyl ether acetate	18.8
Ethyl mercaptan (ethane thiol)	18.8
Propylene oxide	18.8
Propyl formate	18.8
Trichloroethylene	18.8
Tripropylene glycol	18.8
Chloroform	19.0
Dibutyl phthalate	19.0
Methylcyclohexanone	19.0
Methyl ethyl ketone	19.0
Perchloroethylene	19.0
Styrene	19.0
Tetrachloroethylene (perchloroethylene)	19.0
Triphenyl phosphite	19.0
Benzaldehyde	19.2
Butyl lactate (normal)	19.2
Capronitrile (heptyl cyanide)	19.2
Dibenzyl ether	19.2
Dimethyl sulfide	19.2
Ethyl formate	19.2
Ethyl-2-hexanediol-1,3 (octylene glycol)	19.2

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Ethyl iodide (iodoethane)	19.2
Furan	19.2
Nonyl phenol	19.2
Pentachloroethane	19.2
Acetyl chloride	19.2
Chlorobenzene	19.4
Chlorostyrene ( <i>ortho</i> or <i>para</i> )	19.4
Diethylene glycol monobutyl ether (normal)	19.4
Ethylene glycol monobutyl ether	19.4
Ethylhexanol	19.4
Tetrahydronaphthalene (tetralin)	19.4
Ethyl bromide (bromoethane)	19.6
Methyl acetate	19.6
Methyl bromide	19.6
Trichloroethane-1,1,2	19.6
Valeronitrile (normal)	19.6
Chloroethyl acetate ( $\beta$ )	19.8
Dimethylaniline	19.8
Ethylene bromide	19.8
Methyl chloride	19.8
Methylene chloride	19.8
Methyl-2-pentanediol-2,4	19.8
Tetrachloroethane-1,1,2,2	19.8
Dodecanol-1	20-21
Acrolein	20.1
Bromostyrene ( <i>ortho</i> )	20.1
Butyronitrile (iso)	20.1
Dichloroethyl ether	20.1
Ethylene dichloride (1,2-dichloroethane)	20.1
Phenanthrene	20.1
Thiophene	20.1
Valeric acid (normal)	20.1
Acetone	20.3
Anthracene	20.3
Bromobenzene	20.3
Cyclohexanone	20.3
Diethylacetamide ( <i>N,N</i> )	20.3
Diethyl maleate	20.3
Diethyl-2,2-propanediol-1,2 (heptylene glycol)	20.3
Dimethyl carbonate	20.3
Naphthalene	20.3
Nitro-2-propane	20.3
Propionic acid	20.3
Tetraethylene glycol	20.5
Amyl alcohol	20.5
Carbon disulfide	20.5
Dichlorobenzene ( <i>ortho</i> )	20.5
Diethyl phthalate	20.5
Dimethyl-2,2-butanediol-1,3	20.5
Dipentene	20.5
Dipropyl phthalate	20.5
Ethylamine	20.5
Ethylene glycol diacetate	20.5
Ethyl lactate	20.5
Methyl isobutyl carbinol	20.5
Nitrobenzene	20.5
Propionic anhydride	20.7
Acetic acid	20.7
Caprolactone ( $\epsilon$ )	20.7
Dibromoethylene-1,2 ( <i>cis</i> and <i>trans</i> )	20.7
Dipropylene glycol	20.7
Iodobenzene	20.7
Propylene glycol methyl ether (1,2-dimethoxypropane)	20.9
Cresol ( <i>meta</i> )	20.9
Diethylene glycol monobutyl ether	20.9

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Diphenyl ether	20.9
Methyl formate	20.9
Methyl iodide	20.9
Acetaldehyde	21.1
Acetic anhydride	21.1
Aniline	21.1
Butyric acid (iso) (2-methylpropionic acid)	21.1
Methyl-2-pentanediol-1,3	21.1
Nitro-1-propane	21.1
Octyl alcohol (normal)	21.1
Hexanediol-2,5	21.2
Cyclopentanone	21.3
Dibromoethane-1,2	21.5
Acrylonitrile	21.5
Butyl alcohol (iso) (2-methyl-1-propanol)	21.5
Butyric acid (normal)	21.5
Butyronitrile (normal)	21.5
Ethyl-2-butanol-1	21.5
Ethylene glycol monoethyl ether (2-ethoxyethanol; Cellusolve)	21.5
Hexamethylphosphoramide	21.5
Methyl benzoate	21.5
Styrene oxide	21.5
Acetophenone	21.7
1-Bromonaphthalene	21.7
tert-Butyl alcohol (2-methyl-2-propanol)	21.7
Diethylformamide ( <i>N,N</i> )	21.7
Heptyl alcohol (normal)	21.7
Methyl salicylate	21.7
Dimethyl phthalate	21.9
Hexyl alcohol (normal)	21.9
Pyridine	21.9
Triethylene glycol	21.9
sec-Butyl alcohol (2-butanol)	22.1
Dimethylacetamide ( <i>N,N</i> )	22.1
Morpholine	22.1
Pantanediol-2,4	22.1
Propionitrile	22.1
Quinoline	22.1
Quinoline (normal)	22.3
Ethylene glycol monobenzyl ether	22.3
Cyclobutanedione	22.5
Dichloroacetic acid	22.5
Dimethyl malonate	22.5
Dimethyl oxalate	22.5
Epichlorohydrin	22.5
Ethyl cyanoacetate	22.5
Neopentyl glycol	22.5
2,3-Butanediol	22.7
Ethylene oxide	22.7
Nitroethane	22.7
Triethylenetetramine	22.7
Acetylpiridine ( <i>N</i> )	22.7
Dimethyl-2,2-butanediol-1,2 (isobutylene glycol)	22.9
Furfural (2-furaldehyde)	22.9
Methacrylic acid	22.9
Methylamine	22.9
Dipropyl sulfone	22.9
Methyl pyrrolidone-2 (1-methyl-2-pyrrolidinone)	23.1
Acetylpyrrolidine-2 (1-methyl-2-pyrrolidinone)	23.1
n-Butyl alcohol (1-butanol)	23.3
Cyclohexanol	23.3
Ethylene glycol monomethyl ether (2-methoxyethanol)	23.3
Tetramethyloxamide	23.3
Ethylene glycol monophenyl ether	23.5
Formylpiperidine (normal)	23.5

TABLE 8. cont'd

Solvent	$\delta$ (MPa $^{1/2}$ )
Pantanediol-1,5	23.5
Propyl alcohol (2-propanol)	23.5
Acetylmorpholine ( <i>N</i> )	23.7
1,3-Butanediol	23.7
Tolylene diisocyanate (4-methyl-1,3-phenylene diisocyanate)	23.7
Allyl alcohol	24.1
Methylene iodide	24.1
Acetonitrile	24.3
Propyl alcohol (1-propanol)	24.3
Santicizer 8	24.3
Acrylic acid	24.6
Dimethyltetramethylene sulfone	24.6
Benzyl alcohol	24.8
1,4-Butanediol	24.8
Butylene-2,3 carbonate	24.8
Diethylene glycol	24.8
Dimethylformamide ( <i>N,N</i> )	24.8
Diethyl phthalate	24.8
Formic acid	24.8
Hydrogen cyanide	24.8
Ethylene chlorhydrin (2-chloroethanol)	25.0
Ethylacetamide (normal)	25.2
Ethylenediamine	25.2
Diethyl sulfone	25.4
Methylene glycolate	25.4
Dimethyl phosphite	25.6
Furfuryl alcohol	25.6
Methyl propyl sulfone	25.6
Phenylhydrazine	25.6
Butyrolactone ( $\gamma$ )	25.8
Chloroacetonitrile	25.8
Propylene glycol (1,2-propanediol)	25.8
Caprolactam ( $\epsilon$ )	26.0
Ethyl alcohol	26.0
Nitromethane	26.0
Methyltetramethylene sulfone	26.4
Formylmorpholine ( <i>N</i> )	26.6
Dimethylnitroamine ( <i>N,N</i> )	26.8
Propiolactone	27.2
Propylene-1,2-carbonate	27.2
Methyl ethyl sulfone	27.4
Pyrone ( $\gamma$ )	27.4
Tetramethylene sulfone (sulfolane, tetrahydrothiophene 1,1-dioxide)	27.4
Maleic anhydride	27.8
Piperidone	27.8
Diacetyl piperazine ( <i>N,N</i> )	28.0
Ethylene formamide ( <i>N</i> )	28.4
Dimethyl sulfoxide	29.7
Methanol	29.7
Ethylene glycol	29.9
Methylacetamide	29.9
Ethylene carbonate	30.1
Pyrrolidine ( $\alpha$ )	30.1
Malononitrile	30.9
Ethylene cyanohydrin (3-hydroxypropionitrile)	31.1
Diformylpiperazine ( <i>N,N</i> )	31.5
Succinic anhydride	31.5
Methylformamide ( <i>N</i> )	32.9
Ammonia	33.4
Glycerol	33.8

TABLE 9. HANSEN SOLUBILITY PARAMETERS OF LIQUIDS AT 25°C

Solvent	CAS Number	Molar volume (cm <sup>3</sup> /mol)	Solubility parameters (MPa <sup>1/2</sup> )			
			$\delta_d$	$\delta_p$	$\delta_h$	$\delta$
<b>9.1. PARAFFINIC HYDROCARBONS</b>						
n-Butane	106-97-8	101.4	14.1	0	0	14.1
n-Pentane	109-66-0	116.2	14.5	0	0	14.5
Pentane (iso)	78-78-4	117.4	13.7	0	0	14.5
n-Hexane	110-54-3	147.4	14.9	0	0	13.7
n-Heptane	142-82-5	147.4	15.3	0	0	14.9
n-Octane	111-65-9	163.5	15.6	0	0	15.3
2,2,4-Trimethylpentane	540-84-1	166.1	14.3	0	0	15.6
n-Nonane	111-84-2	179.7	15.8	0	0	14.3
n-Decane	124-18-5	195.9	15.8	0	0	15.8
n-Dodecane	112-40-3	228.6	16	0	0	16
n-Hexadecane	544-76-3	294.1	16.4	0	0	16.4
n-Eicosane	112-95-8	359.8	16.6	0	0	16.6
Cyclohexane	110-82-7	108.7	16.8	0	0.2	16.8
Methylcyclohexane	108-87-2	128.3	16	0	1	16
cis-Decahydronaphthalene	493-01-6	156.9	18.8	0	0	18.8
trans-Decahydronaphthalene	493-02-7	159.9	18.8	0	0	18.8
<b>9.2. AROMATIC HYDROCARBONS</b>						
Benzene	71-43-2	89.4	18.4	0 <sup>a</sup>	2	18.6
Toluene	108-88-3	106.8	18	1.4	2	18.2
Naphthalene <sup>b</sup>	91-20-3	111.5	19	2	5.9	20
Styrene	1-42-5	115.6	18.6	1	4.1	19
<i>o</i> -Xylene	95-47-6	121.2	17.8	1	3.1	18
Ethylbenzene	1-41-4	123.1	17.8	0.6	1.4	17.8
1-Methylnaphthalene	90-12-0	138.8	20.6	0.8	4.7	21.2
Mesitylene	108-67-8	139.8	18	0	0.6	18
Tetrahydronaphthalene	119-64-2	136.0 <sup>a</sup>	19.6 <sup>a</sup>	0	2.9	20
Biphenyl	92-52-4	154.1	21.5	1	2	21.7
<i>p</i> -Diethylbenzene	105-05-5	156.9	18	0	0.6	18
<b>9.3. HALOHYDROCARBONS</b>						
Methyl chloride	74-87-3	55.4	15.3	6.1	3.9	17
Methylene dichloride	75-09-2	63.9	18.2	6.3	6.1	20.3
Bromoform	74-97-5	65	17.4	5.7	3.5	18.6
Chlorodifluoromethane	75-45-6	72.9	12.3	6.3	5.7	14.9
Dichlorofluoromethane	75-43-4	75.4	15.8	3	5.7	17
Ethyl bromide	74-96-4	76.9	16.6	8	5.1	19
1,1-Dichloroethylene	75-35-4	79	17	6.8	4.5	18.8
Ethylene dichloride	107-06-2	79.4	19.0 <sup>a</sup>	7.4	4.1	20.9
Methylene diiodide <sup>c</sup>	75-11-6	80.5	17.8	3.9	5.5	19
Chloroform	67-66-3	80.7	17.8	3.1	5.7	19
1,1-Dichloroethane	75-34-3	84.8	16.6	8.2	0.4	18.4
Ethylene dibromide	106-93-4	87	19.6	6.8	12.1	23.9
Bromoform	75-25-2	87.5	21.5 <sup>a</sup>	4.1	6.1 <sup>a</sup>	22.7
<i>n</i> -Propyl chloride	540-54-5	88.1	16	7.8	2	17.8
Trichloroethylene	79-01-6	90.2	18	3.1	5.3	19
Dichlorodifluoromethane	75-71-8	92.3	12.3	2	0	12.5
Trichlorofluoromethane	75-69-4	92.8	15.3	2	0	15.5
Bromotrifluoromethane	75-63-8	97	9.6	2.5	0	10
Carbon tetrachloride	56-23-5	97.1	17.8	0	0.6	17.8
1,1,1-Trichloroethane	71-55-6	1.4	17	4.3	2	17.6
Tetrachloroethylene	127-18-4	101.1	19	6.5 <sup>a</sup>	2.9 <sup>a</sup>	20.3
Chlorobenzene	108-90-7	102.1	19	4.3	2	19.6
<i>n</i> -Butylchloride	109-69-3	104.9	16.4	5.5	2	17.4
1,1,2,2-Tetrachloroethane	79-34-5	105.2 <sup>a</sup>	18.8	5.1	9.4	21.7
Bromobenzene	222-22-2	105.3	20.5	5.5	4.1	21.7
<i>o</i> -Dichlorobenzene	95-50-1	112.8	19.2	6.3	3.3	20.5
Benzyl chloride	100-44-7	115	18.8 <sup>a</sup>	7.2	2.7	20.3
1,1,2,2-Tetrabromoethane <sup>c</sup>	79-27-6	116.8	22.7	5.1	8.2	24.8
1,2-Dichlorotetrafluoroethane <sup>c</sup>	76-14-2	117	12.7	1.8	0	12.9
1,1,2-Trichlorotrifluoroethane	76-13-1	119.2	14.7	1.6	0	14.7
Cyclohexyl chloride	542-18-7	121.3	17.4	5.5	2	18.4

TABLE 9. cont'd

Solvent	CAS Number	Molar volume (cm <sup>3</sup> /mol)	Solubility parameters (MPa <sup>1/2</sup> )			
			$\delta_d$	$\delta_p$	$\delta_h$	$\delta$
<b>9.4. ETHERS</b>						
1-Bromonaphthalene	90-11-9	140	20.3	3.1	4.1	20.9
Trichlorobiphenyl <sup>d</sup>	7012-37-5	187	19.2	5.3	4.1	20.5
Perfluoromethylcyclohexane	355-02-2	196	12.5	0	0	12.5
Perfluorodimethylcyclohexane	335-27-3	217.4	12.5	0	0	12.5
Perfluoro- <i>n</i> -heptane	335-57-9	227.3	12.1	0	0	12.5
<b>9.5. KETONES</b>						
Acetone	67-64-1	74	15.5	10.4	7	20.1
Methyl ethyl ketone (2-butanone)	78-93-3	90.1	16	9	5.1	19
Cyclohexanone	108-94-1	104	17.8	6.3	5.1	19.6
Diethyl ketone (3-pentanone)	96-22-0	106.4	15.8	7.6	4.7	18.2
Methyl oxide (4-methyl-3-pentene-2-one)	141-79-7	115.6	16.4	7.2	6.1	18.8
Acetophenone	98-86-2	117.4	19.6 <sup>a</sup>	8.6	3.7	21.7
Methyl iso-butyl ketone (2-hexanone)	591-78-6	125.8	15.3	6.1	4.1	17
Methyl iso-amyl ketone		142.8	16	5.7	4.1	17.4
Isophorone	78-59-1	150.5	16.6	8.2	7.4	19.8
Di-iso-butyl ketone (2,6-dimethyl-4-heptanone)	108-83-8	177.1	16	3.7	4.1	16.8
<b>9.6. ALDEHYDES</b>						
Acetaldehyde	75-07-0	57.1	14.7	8	11.3	20.3
2-Furfuraldehyde (furfural)	98-01-1	83.2	18.6	14.9	5.1	24.3
Butyraldehyde	123-72-8	88.5	14.7	5.3	7	17.2
Benzaldehyde	100-52-7	101.5	19.4	7.4	5.3	21.5
<b>9.7. ESTERS</b>						
Ethylene carbonate (1,3-dioxolan-2-one)	96-41-9	66	19.4	21.7	5.1	29.5
$\gamma$ -Butyrolactone (4-hydroxybutyric acid $\gamma$ -lactone)	96-48-0	76.8	19	16.6	7.4	26.2
Methyl acetate	79-20-9	79.7	15.5	7.2	7.6	18.8
Ethyl formate	109-94-4	80.2	15.5	8.4	8.4	19.6
Propylene carbonate (1,2-propanediol cyclic carbonate)	108-32-7	85	20.1	18	4.1	27.2
Ethyl chloroformate	541-41-3	95.6	15.5	10	6.8	19.6
Ethyl acetate	141-78-6	98.5	15.8 <sup>a</sup>	5.3	7.2 <sup>a</sup>	18.2
Trimethyl phosphate	512-56-1	99.9	16.8	16	10.2	25.4

TABLE 9. cont'd

Solvent	CAS Number	Molar volume (cm <sup>3</sup> /mol)	Solubility parameters (MPa <sup>1/2</sup> )			
			$\delta_d$	$\delta_p$	$\delta_h$	$\delta$
Iso-propyl palmitate <sup>c</sup>	2239-78-3	330	14.3	3.9	3.7	15.3
Di-n-butyl sebacate	109-43-3	339	14.5	3.9	3.7	15.5
Methyl oleate <sup>d</sup>	112-62-9	340	14.5	3.9	3.7	15.5
Diocyl phthalate (bis(2-ethylhexyl) phthalate)	117-81-7	377	16.6	7	3.1	18.2
Di-butyl stearate <sup>c</sup>		382	14.5	3.7	3.5	15.3
<b>9.8. NITROGEN-CONTAINING COMPOUNDS</b>						
Acetonitrile	75-05-8	52.6	15.3	18	6.1	24.6
Acrylonitrile	107-13-1	67.1	16.5	17.4	6.8	24.8
Propionitrile	107-12-0	70.9	15.3	14.3	5.5	21.7
Butyronitrile	109-74-0	87	15.3	12.5	5.1	20.5
Benzonitrile	100-47-0	102.6	17.4	9	3.3	19.8
Nitromethane	75-52-5	54.3	15.8	18.8	5.1	25
Nitroethane	79-24-3	71.5	16	15.5	4.5	22.7
2-Nitropropane	79-46-9	86.9	16.2	12.1	4.1	20.7
Nitrobenzene	98-95-3	102.7	20.1	8.6	4.1	22.1
Ethanolamine (2-aminoethanol)	141-43-5	60.2	17.2	15.5	21.3	31.5
Ethylene diamine	107-15-3	67.3	16.6	8.8	17	25.4
1,1-Dimethylhydrazine <sup>c</sup>	57-14-7	76	15.3	5.9	11	19.8
2-Pyrrolidone (2-pyrrolidinone)	616-45-5	76.4	19.4	17.4	11.3	28.4
Pyridine	110-86-1	80.9	19	8.8	5.9	21.7
n-Propylamine	107-10-8	83	17	4.9	8.6	19.6
Morpholine	110-91-8	87.1	18.8	4.9	9.2	21.5
Aniline	62-53-3	91.5	19.4	5.1	10.2	22.5
N-Methyl-2-pyrrolidone (1-methyl-2-pyrrolidinone)	872-50-4	96.5	18	12.3	7.2	22.9
n-Butylamine	109-73-9	99	16.2 <sup>a</sup>	4.5 <sup>a</sup>	8	18.6
Diethylamine	109-87-7	103.2	14.9	2.3	6.1	16.4
Diethylenetriamine	111-40-0	108	16.8	13.3	14.3	25.8
Cyclohexylamine	108-91-8	115.2	17.4	3.1	6.5	18.8
Quinoline	91-22-5	118	19.4	7	7.6	22.1
Di-n-propylamine	142-84-7	136.9	15.3	1.4	4.1	16
Formamide	75-12-7	39.8	17.2	26.2	19	36.6
Dimethylformamide	68-12-2	77	17.4	13.7	11.3	24.8
N,N-Dimethylacetamide	127-19-5	92.5	16.8	11.5	10.2	22.7
1,1,3,3-Tetramethylurea	632-22-4	120.4	16.8	8.2	11	21.7
Hexamethyl phosphoramide <sup>c</sup> (hexamethyl phosphoric triamide)	680-31-9	175.7	18.4	8.6	11.3	23.3
<b>9.9. SULFUR-CONTAINING COMPOUNDS</b>						
Carbon disulfide	75-15-0	60	20.5	0	0.6	20.5
Dimethyl sulfoxide (methyl sulfoxide)	67-68-5	71.3	18.4	16.4	10.2	26.6
Ethanethiol <sup>c</sup> (ethyl mercaptan)	75-08-1	74.3	15.8	6.5	7.2	18.4
Dimethyl sulfone <sup>b</sup> (methyl sulfone)	67-71-0	75	19	19.4	12.3	29.9
Diethyl sulfide (ethyl sulfide)	352-93-2	108.2	17	3.1	2	17.4
<b>9.10. ACID HALIDES AND ANHYDRIDES</b>						
Acetyl chloride	75-36-5	71	15.8	10.6	3.9	19.4
Succinic anhydride <sup>b</sup>	108-30-5	66.8	18.6	19.2	16.6	31.5
Acetic anhydride	108-24-7	94.5	16.0 <sup>a</sup>	11.7 <sup>a</sup>	10.2 <sup>a</sup>	22.3
<b>9.11. ALCOHOLS</b>						
Methanol	67-56-1	40.7	15.1	12.3	22.3	29.7
Ethanol	64-17-5	58.5	15.8	8.8	19.4	26.6
Ethylene cyanohydrin (hydracylonitrile; 3-hydroxypropionitrile)	109-78-4	68.3	17.2	18.8	17.6	30.9
Allyl alcohol (2-propen-1-ol)	107-18-6	68.4	16.2	10.8	16.8	25.8
1-Propanol	71-23-8	75.2	16	6.8	17.4	24.6
2-Propanol	67-63-0	76.8	15.8	6.1	16.4	23.5
3-Chloropropanol (trimethylene chlorohydrin)	627-30-5	84.2	17.6	5.7	14.7	23.7
Furfuryl alcohol	98-00-0	86.5	17.4	7.6	15.1	24.3
1-Butanol (butyl alcohol)	71-36-3	91.5	16	5.7	15.8	23.1
2-Butanol	4221-99-2	92	15.8	5.7	14.5	22.1

TABLE 9. cont'd

Solvent	CAS Number	Molar volume (cm <sup>3</sup> /mol)	Solubility parameters (MPa <sup>1/2</sup> )			
			$\delta_d$	$\delta_p$	$\delta_h$	$\delta$
2-Methyl-1-propanol (isobutyl alcohol)	78-83-1	92.8	15.1	5.7	16	22.7
Benzyl alcohol	100-51-6	103.6	18.4	6.3	13.7	23.7
Cyclohexanol <sup>b</sup>	108-93-0	106	17.4	4.1	13.5	22.5
1-Pentanol <sup>b</sup>	71-41-0	109	16	4.5	13.9	21.7
2-Ethyl-1-butanol	97-95-0	123.2	15.8	4.3	13.5	21.3
Diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)	123-42-2	124.2	15.8	8.2	10.8	20.9
1,3-Dimethyl-1-butanol	105-30-6	127.2	15.3	3.3	12.3	19.8
Ethyl lactate	687-47-8	115	16	7.6	12.5	21.7
n-Butyl lactate	138-22-7	149	15.8	6.5	10.2	19.8
Ethylene glycol monomethyl ether (2-methoxyethanol)	109-86-4	79.1	16.2	9.2	16.4	24.8
Ethylene glycol monoethyl ether (2-ethoxyethanol) Cellusolve	111-15-9	97.8	16.2	9.2	14.3	23.5
Diethylene glycol monomethyl ether (2-(2-methoxyethoxy)ethanol)	111-77-3	118	16.2	9.2	12.3	22.3
Diethylene glycol monoethyl ether (2-(2-ethoxyethoxy)ethanol)	111-90-0	130.9	16.2	9.2	12.3	21.9
Ethylene glycol mono-n-butyl ether (2-butoxyethanol) Butyl Cellusolve	111-76-2	131.6	16	5.1	12.3	22.3
2-Ethyl-1-hexanol	104-76-7	157	16	3.3	11.9	20.1
1-Octanol (capryl alcohol)	111-87-5	157.7	17	3.3	11.9	20.9
2-Octanol	123-96-6	159.1	16.2	4.9	11	20.3
Diethylene glycol mono-n-butyl ether (2-(2-butoxyethoxy)ethanol)	112-34-5	170.6	16	7	10.6	20.5
1-Decanol	112-30-1	191.8	17.6	2.7	10	20.5
Tridecyl alcohol <sup>d</sup>	112-70-9	242	14.3	3.1	9	17.2
Nonyl phenoxy ethanol <sup>d</sup>	27986-36-3	275	16.8	10.2	8.4	21.3
Oleyl alcohol <sup>d</sup>	143-28-2	316	14.3	2.7	8	16.6
Triethylene glycol mono-oleyl ether	418.5	13.3	3.1	8.4	16	
<b>9.12. ACIDS</b>						
Formic acid	64-18-6	37.8	14.3	11.9	16.6	25
Acetic acid	64-19-7	57.1	14.5	8	13.5	21.3
Benzoic acid <sup>b</sup>	65-85-0	100	18.2	7	9.8	21.9
n-Butyric acid <sup>c</sup>	107-92-6	110	14.9	4.1	10.6	18.8
n-Octanoic acid <sup>c</sup>	124-07-2	159	15.1	3.3	8.2	17.6
Oleic acid	112-80-1	320	14.3	3.1	5.5	15.8
Stearic acid <sup>b</sup>	57-11-4	326	16.4	3.3	5.5	17.6
<b>9.13. PHENOLS</b>						
Phenol	108-95-2	87.5	18	5.9	14.9	24.1

TABLE 10. SOLUBILITY PARAMETERS OF POLYMERS

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Ref.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$			
<b>10.1. MAIN CHAIN CARBON POLYMERS</b>								
10.1.1. POLY(DIENES)								
Poly(butadiene)								
Emulsion					14.65	Calc.		
Sodium					17.19			28
Hydrogenated					17.09			66
					17.15	Calc.		110
					17.2–17.6	Obs.		112
					16.6			112
					17.6			118
					16.2 ± 0.2	IPGC	75	72
					17.19			70
					17.6			79
					16.6	Calc.		62
					17.09			104
					16.6	Swelling		75
					16.47			75
					16.6	Av.		75
		16.98	— <sup>a</sup>	1.02	17.02			98
Poly(1,2-butadiene)	58.85				16.1	<sup>129</sup> Xe shift		152
Poly(3-methyl 1,2-butadiene)	73.88				17.06	Calc. <sup>HK<sup>b</sup></sup>		3
Poly(1,3-butadiene)	58.85				17.39	Calc. <sup>HK</sup>		3
Poly(2,3-dimethyl 1,3 butadiene)	88.91				17.06	Calc. <sup>HK</sup>		3
Poly( <i>cis</i> -butadiene) elastomer (Bunahyls CB10, Chemische Werke Huels)	17.53		2.25	3.42	17.60	Calc. <sup>HK</sup>		3
Poly(butadiene- <i>co</i> -acrylonitrile)					18			56
BUNA N (82/18)					17.90–17.72			19
(82/20)					18.4	Calc.		66
BUNA N (75/25)					19.4	Obs.		66
					18.93	Calc.	25	112
					19.19	Obs.		42
					19.4	Obs.		104
					18.2			118
					19.4			79
(70/30)					20.11–20.26			19
					19.19			43
					21.1			19
					21.28–21.38			19
					20.5 ± 0.6	IPGC	75	70
Hycar (BFGoodrich)	18.6		8.8	4.2	21			56
Poly(butadiene- <i>co</i> -styrene)								
BUNA S (94/6)					16.45–16.64			19
(90/10)					17.13			110
(87.5/12.5)					16.39–16.57			19
					16.55			43
					17.6			104
					17.31			112
					17.19			110
					17.35	Calc.		112
					17.4	Obs.		79
					17.39			66
					17.41	Calc.		66
					17.39	Obs.		104
					17.5			110
					17.29			112
					17.47	Calc.		112
					16.55	Obs.		112
					16.49	Obs.		118
					16.6			79
					17.5			66
					17.56	Calc.		66
					17.5	Obs.		104
					17.6			104

TABLE 10. *cont'd*

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Refs.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$			
(71.5/28.5)					16.55–16.72			19
					17.51			112
					17.35			110
(70/30)					17.5			110
(60/40)					17.7	Calc.		112
					17.74	Obs.		112
					17.74			79
					17.76	Calc.		66
					17.74	Obs.		66
					17.8			104
					18.07			56
Poly(butadiene- <i>co</i> -styrene) (Polysar 5630, Polymer Corp.)	17.55	3.36	2.7					79
Poly(butadiene- <i>co</i> -vinylpyridine)					19.13			25
Poly(chloroprene)					18.42			110
					16.59	Calc.		28
					19.19	Calc.		112
					16.74	Obs.		42
					18.93	Obs.		104
					17.6			118
					16.8			44
					18.8			72
					16.6			79
					17.6	Swelling		43
					17.54–17.74			19
					15.18			19
					18.0 ± 0.4	IPGC	75	70
					17.6	<sup>129</sup> Xe shift		152
					15.18	Calc.	25	28
Poly(1,4- <i>cis</i> -isoprene)					16.64			42
					16.68			25
					16.57			74
					20.46	Swelling	35	74
					16.47	Av.	35	74
					16.47	Swelling	35	74
					16.57	Swelling	35	74
					16.68	Calc.	35	74
					16.6	Swelling		75
					16.4			76
					16.47	Av.		76
					16.82			25
					16.68	Calc.	25	110
					16.2	Obs.		112
					16.33	Obs.		112
					17.09	Obs.		112
					16.2			72
Poly(isoprene) elastomer (Cariflex IR 305, Shell) Natural Rubber	16.57	1.41	– 0.82		16.65			56
					16.2			43
					16.6			19
					16.68			112
					17.09			104
					17			124
					16.6			118
					16.4			19,10
					17.09			79
					16.33			43
					16.6			19
					16.42–16.49			19
					16.2	<sup>129</sup> Xe shift		152
					16.6	Calc.		73
Gutta percha Chlorinated					19.2			21–24
10.1.2. POLY(ALKENES)								
Poly(2,3-dimethyl 1-butene)	93.15				18.05	Calc. <sup>HK</sup>		
Poly(3,3-dimethyl 1-butene)	93.15				18.05	Calc. <sup>HK</sup>		

TABLE 10. *cont'd*

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Ref.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$			
Poly(3-methyl 1-butene)	78.12				17.76	Calc. <sup>HK</sup>		
Poly(2-methyl 1-butene)	78.12				17.92	Calc. <sup>HK</sup>	3	
Poly(2-methyl 2-butene)	78.12				17.68	Calc. <sup>HK</sup>	3	
Polyethylene					15.76		3	
					16.6	Calc.	110	
					16		112	
					16.2		58	
					17.09		97	
					16.4	Calc.	8	
					16.2		124	
					16.2		118	
					16.8	Calc.	72	
					16.2	Obs.	97	
					18.4	<sup>129</sup> Xe shift	73	
					17.99	Calc.	152	
					16.96	Calc. <sup>HK</sup>	119	
					19.93	Calc. <sup>HK</sup>	3	
					14.3	Extrapol.	20	45
					18.6 ± 0.9	IPGC	25	71
					17.0 ± 0.4	IPGC	75	70
					14.5	Calc.	28	
					16.06	Av.	35	74
					16	Swelling	74	
					16.47	Swelling	74	
					16.25		19,10	
					16.06		110	
					15.76	Calc.	112	
					16.47	Obs.	112	
					16.4		58	
					16.47		104	
					16.6		21-24	
					16		19	
					17	Calc.	124	
					16.47		72	
					16.47		79	
					15.47		56	
					15	<sup>129</sup> Xe shift	152	
					15.9–16.06		19	
					16.47		104	
					15.76		112	
					18.8		58	
					19.2	Calc.	124	
					17.49	Calc. <sup>HK</sup>	3	
					17.19		81	
					21.89		56	
					17.72	Calc. <sup>HK</sup>	3	
					18		35	
					18.01	Av.	75	
					18.52	Swelling	75	
					17.4	Calc.	75	
					18.6	Swelling	77	
					18.52		77	
					19.77	Calc.	119	
					19.13	Av.	75	
					19.2	Swelling	75	
					19.8	Calc.	77	
					19.2	Swelling	77	
					19.13		45	
					19.19		62	
					18.8	Calc.	119	
					20.4	Calc.	119	
Poly(acrylic acid), butyl ester								
Poly(acrylic acid), ethyl ester								

TABLE 10. *cont'd*

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Refs.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$			
Poly(acrylic acid), isobornyl ester								16.8
Poly(acrylic acid), methyl ester								20.7
Poly(acrylic acid), propyl ester								20.77
Poly( $\alpha$ -chloroacrylic acid), methyl ester								20.1
Poly(methacrylic acid), butyl ester								20.77
Poly(methacrylic acid), isobutyl ester								21.3
Poly(methacrylic acid), <i>sec</i> -butyl ester								20.7
Poly(methacrylic acid), ethoxyethyl ester								18.52
Poly(methacrylic acid), ethyl ester								18.42
Poly(ethyl methacrylate) (Lucite 2042, DuPont)		18.64	10.52	7.51	22.69			152
					20.4	<sup>129</sup> Xe shift		73
					17.6	Calc.		62
					16.6			73
					16.8	Calc.	25	19
					18.52–18.66			19
					19.4	Swelling		77
					19.34			77
					26.27			110
					18.93	Calc.		112
					18.4			7
					18.2			118
					18.6	Calc.		119
					22.69			56
					20.4			73
					17.2			73
					18			73
					16			118
					21			112
					21.9	Calc.		112
					25.78			110
					21.7			139
					22.5			139
10.1.4. POLY(VINYL ALCOHOLS)								
Poly(vinyl alcohol)								
Poly(4-vinyl phenol)								
10.1.5. POLY(VINYL ESTERS)								
Poly(vinyl acetate)								
								19.62
								19.13
								20.93
								19.2
								18
								22.61
								19.2
								19.2
								56
								25
								110
								112
								118
								56
								119
								35
								78
Poly(vinyl acetate) (Mowilith 50, Hoechst)		20.93	11.27	9.66	25.66			
Poly(vinyl acetate- <i>co</i> -vinyl alcohol)					21.94			
Poly(vinyl butyral) (Butvar B76, Shawinigan)		18.6	4.36	13.03	23.12			
Poly(vinyl propionate)					18.01			
					18.52			
					Calc.			

TABLE 10. cont'd

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>					Method	T(°C)	Refs.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$				
<b>10.1.6. POLY(ALLYL ETHERS) AND POLY(VINYL ETHERS)</b>									
Poly(allyl methyl ether)	70.79				19.44	Calc. HK			3
Poly(allyl ethyl ether)	85.82				19.29	Calc. HK			3
Poly(allyl propyl ether)	100.85				19.21	Calc. HK			3
Poly(allyl isopropyl ether)	100.85				19.21	Calc. HK			3
Poly(allyl phenyl ether)	122.39				20.19	Calc. HK			3
Poly(allyl 2, tolyl ether)	137.41				20.03	Calc. HK			3
Poly(allyl 3, tolyl ether)	137.41				20.03	Calc. HK			3
Poly(allyl 4, tolyl ether)	137.41				20.03	Calc. HK			3
Poly(diallyl ether)	96.61				18.84	Calc. HK			3
Poly(vinyl methyl ether)	55.76				19.66	Calc. HK			3
Poly(vinyl ethyl ether)	70.79				19.44	Calc. HK			3
Poly(vinyl propyl ether)	85.82				19.29	Calc. HK			3
Poly(vinyl butyl ether)	100.85				19.21	Calc. HK			3
Poly(vinyl isopropyl ether)	85.82				19.29	Calc. HK			3
Poly(vinyl isobutyl ether)	100.85				19.21	Calc. HK			3
Poly(vinyl isoamyl ether)	115.88				19.13	Calc. HK			3
Poly(vinyl-1-amyl methyl ether)	119.91				20.83	Calc. HK			3
Poly(vinyl-2-ethyl hexyl ether)	160.96				18.99	Calc. HK			3
Poly(vinyl-2-methoxyethyl ether)	93.52				20.44	Calc. HK			3
Poly(vinyl phenyl ether)	107.36				20.19	Calc. HK			3
Poly(vinyl-1-phenyl methyl ether)	122.39				20.19	Calc. HK			3
Poly(vinyl-1-methyl phenyl ether)	122.39				20.19	Calc. HK			3
Poly(vinyl-1-phenyl phenyl ether)	174.01				20.50	Calc. HK			3
Poly(1-methyl vinyl ethyl ether)	85.82				19.29	Calc. HK			3
Poly(1-ethyl vinyl ethyl ether)	100.85				19.21	Calc. HK			3
Poly(1-phenyl vinyl ethyl ether)	137.41				20.03	Calc. HK			3
Poly(divinyl ether)	66.55				18.93	Calc. HK			3
<b>10.1.7. POLY(VINYL HALIDES) AND POLY(VINYL NITRILES)</b>									
Poly(acrylonitrile)					25.27	Calc.	119		
					25.6		66		
					26.09	Calc.	25	112	
					31.5		118		
					18.21	16.16	6.75	98	
Poly(allyl acetonitrile)	81.13				25.27	Calc. HK			
Poly(1-methyl acrylonitrile)	66.09				24.18	Calc. HK			
Poly(2-methyl acrylonitrile)	66.09				25.45	Calc. HK			
Poly(acrylonitrile- <i>co</i> -isopropyl methacrylate)					19.84		141		
Poly(tetrafluoroethylene)					12.7	Calc.	112		
Poly(vinyl bromide)					12.7		118		
Poly(vinyl chloride)					19.42		34		
Poly(vinyl chloride) (Vipla KR, K = 50, Montecatini)	18.23	7.53	8.35	21.42			112		
Poly(vinyl chloride)	18.72	10.03	3.07	21.46			19		
Poly(vinyl chloride), high molecular weight	18.82	10.03	3.07	21.54			28		
Poly(vinyl chloride), chlorinated					20.13	Turbidity	112		
					20.25	Swelling	162		
					20.3	Visc.	162		
					19	Visc.	162		
							117		
							25		

TABLE 10. cont'd

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>					Method	T(°C)	Refs.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$				
<b>10.1.8. POLY(STYRENES)</b>									
Poly(styrene)									17.52
									17.45–17.58
									20.16
									17.86–17.92
									17.84–18.56
									18.6
									18.72
									18.62
									18.62
									18.66
									19.09
									18.66
									18.6
									17.6–19.8
									17.4
									17.6
									18.4
									19.28
									21.1
									17.52
									17.84
									18.6
									18.6
									15.6
									IPGC
									140
									31
									56
Poly(styrene) (Polystyrene LG, BASF)							21.28	5.75	4.3
									22.47
									19.33
									19.33
									19.33
									19.33
									19.33
									19.33
									20.19
									22.36
									22.71
									22.20
									18.6
									17.39
									14.8
									15.7
									17.8
									15.1
									15.1
									19.02
									16.4
									17.8
									21.7
									24.55

TABLE 10. cont'd

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Refs.
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$			
Poly(4- $\alpha$ -acetoxystyrene), -CH <sub>2</sub> -C-(OCOCH <sub>3</sub> )-(C <sub>6</sub> H <sub>5</sub> -OCOR)-, R=CH <sub>3</sub> , C <sub>2</sub> H <sub>5</sub> , n-C <sub>3</sub> H <sub>7</sub> , OCH <sub>3</sub>	15.7	10.2	7.4	21.9				161
Poly(vinylidene cyanide-co-4- $\alpha$ -acetoxystyrene), -CH <sub>2</sub> -C(CN) <sub>2</sub> -CH <sub>2</sub> -C-(OCOCH <sub>3</sub> )- (C <sub>6</sub> H <sub>5</sub> -OCOR)-, R=CH <sub>3</sub>	21.5	11.3	7.2	25.3				161
Poly(vinylidene cyanide-co-4- $\alpha$ -acetoxystyrene), R=OCOCH <sub>3</sub>	17	13.5	6.5	23.5				161
Poly(vinylidene cyanide-co-4- $\alpha$ -acetoxystyrene), R=OCOCH <sub>3</sub>	17	12.1	8.2	22.4				161
Poly(vinylidene cyanide-co-4- $\alpha$ -acetoxystyrene), R=OCOCH <sub>3</sub>	17	11.9	7.2	21.9				161
<b>10.2. MAIN CHAIN C-O POLYMERS</b>								
10.2.1. POLY(ESTERS)								
Poly(vinyl acetate)	74.25				18.21	Calc. HK	3	
Poly(allyl acetate)	89.28				18.27	Calc. HK	3	
Poly(diethylaminoethyl acrylate)-palladium ion					20.50		136	
Poly(methyl acrylate)	74.25				18.21	Calc. HK	3	
Poly(ethyl acrylate)	89.28				18.27	Calc. HK	3	
Poly(allyl acrylate)	100.07				17.94	Calc. HK	3	
Poly(butyl acrylate)	119.34				20.42	Calc. HK	3	
Poly(isobutyl acrylate)	119.34				18.37	Calc. HK	3	
Poly(2-ethyl hexyl acrylate)	179.46				18.45	Calc. HK	3	
Poly(2-cyanoethyl acrylate) <sup>a</sup>	89.36				31.77	Calc. HK	3	
Poly(benzyl acrylate)	140.88				19.38	Calc. HK	3	
Poly(vinyl butyrate)	104.31				18.33	Calc. HK	3	
Poly(dimethyl citraconate)	130.5				18.58	Calc. HK	3	
Poly(diethyl citraconate)	160.58				18.58	Calc. HK	3	
Poly(vinyl crotonate)	100.07				17.94	Calc. HK	3	
Poly(methyl dimethyl fumarate)	130.5				18.58	Calc. HK	3	
Poly(methyl diethyl fumarate)	160.56				18.58	Calc. HK	3	
Poly(dimethyl fumarate)	115.47				18.56	Calc. HK	3	
Poly(diethyl fumarate)	145.53				18.58	Calc. HK	3	
Poly(dipropyl fumarate)	165.58				19.72	Calc. HK	3	
Poly(di-n-butyl fumarate)	205.65				18.60	Calc. HK	3	
Poly(di-n-amyl fumarate)	235.71				18.60	Calc. HK	3	
Poly(di-isopropyl fumarate)	165.58				19.72	Calc. HK	3	
Poly(di-isobutyl fumarate)	205.65				18.60	Calc. HK	3	
Poly(di-isoamyl fumarate)	235.71				18.60	Calc. HK	3	
Poly(dinitrile fumarate)	46.32				48.45	Calc. HK	3	
Poly(diphenyl fumarate)	217.67				19.91	Calc. HK	3	
Poly(vinyl-2-ethyl hexoate)	157.83				19.21	Calc. HK	3	
Poly(dimethyl maleate)	115.47				18.56	Calc. HK	3	
Poly(diethyl maleate)	145.53				18.58	Calc. HK	3	
Poly(di-n-propyl maleate)	165.58				19.70	Calc. HK	3	
Poly(di-n-butyl maleate)	205.65				18.60	Calc. HK	3	
Poly(di-n-amyl maleate)	235.71				18.60	Calc. HK	3	
Poly(di-isobutyl maleate)	205.65				18.60	Calc. HK	3	
Poly(di-isoamyl maleate)	235.71				18.60	Calc. HK	3	
Poly(diphenyl maleate)	217.67				19.91	Calc. HK	3	
Poly(3-chloropropyl methacrylate)					19.60		160	
Poly(methyl methacrylate)	89.28				18.27	Calc. HK	3	
Poly(ethyl methacrylate)	110.9				17.25	Calc. HK	3	
Poly(propyl methacrylate)	119.34				18.37	Calc. HK	3	
Poly(butyl methacrylate)	134.37				18.41	Calc. HK	3	
Poly(hexyl methacrylate)	191.91				15.80	Calc. HK	3	
Poly(allyl methacrylate)	115.1				17.51	Calc. S	3	
Poly(isopropyl methacrylate)	119.34				18.39	Calc. HK	3	
Poly(isobutyl methacrylate)	134.37				18.39	Calc. HK	3	
Poly(vinyl propionate)	89.32				18.27	Calc. HK	3	

TABLE 10. cont'd

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Refs.				
		$\delta_d$	$\delta_p$	$\delta_h$	$\delta$							
<b>10.3. MAIN CHAIN C-N POLYMERS</b>												
10.3.1. POLY(AMIDES)												
Poly(lactams)												
Nylon 3								26.2 Calc. 139				
Nylon 4								23.9 Calc. 139				
								19.42 81				
								22.5 Calc. 139				
								21.5 Calc. 139				
								20.7 Calc. 139				
								20.3 Calc. 139				
								19.8 Calc. 139				
								19.4 Calc. 139				
								19.2 Calc. 139				
								19 Calc. 139				
								27.2 Calc. 139				
								26 Calc. 139				
								25 Calc. 139				
								24.1 Calc. 139				
								23.5 Calc. 139				
								26.3 Calc. HK 150				
								23.2 Calc. H <sup>d</sup> 150				
								22.9 Calc. 139				
								22.5 Calc. 139				
								22.1 Calc. 139				
								21.7 Calc. 139				
								21.1 Calc. 139				
								98				
								56				
								118				
								56				
								143				
								143				
								143				
								143				
								143				
								110				
								110				
								81				
								81				
								140				
								140				
								110				
								110				
								110				
								112				
								18				
								18				
								112				
								112				
								118</				

TABLE 10. cont'd

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Refs.
		δ <sub>d</sub>	δ <sub>p</sub>	δ <sub>h</sub>	δ			
<b>10.4. OTHER POLYMERS</b>								
Alcohol soluble resin (Pentalyn 255, Hercules)	17.5	9.3	14.3	24.4			56	
Alcohol soluble rosin resin (Pentalyn 830, Hercules)	20	5.8	10.9	23.5			56	
Alkyd, short oil (coconut oil 34% phthalic anhydride, Plexal C34)	18.5	9.21	4.91	21.24			56	
Alkyd resin, medium oil length				19.2			21-24	
Alkyd, long oil (66% oil length, Plexal P65, Polyplex)	20.42	3.44	4.56	12.2			56	
Coumarone-indene resin (Piccoumarone 450L, Penn. Ind. Chem.)	19.42	5.48	5.77	20.99			56	
Epoxy resin				22.3			118	
Epoxy (Epikote 1001, Shell)	20.36	12.03	11.48	26.29			56	
Epoxy DBEBA-DDMe*	32			22			56	
DGEBA-DMM	22			22.2			35	
TGAP-DDMe	22.4			22.5			35	
TGAP-ANI				23.9			35	
TGAP-DDM				24.8			35	
TGAP-DDS				27.1			35	
Ester gum (ester gum BL, Hercules)	19.64	4.73	7.77	21.65			56	
Furfuryl alcohol resin (Durez 14383, Hooker Chemical)	21.16	13.56	12.81	28.21			56	
Hexamethoxymethyl melamine (Cymel 300, American Cyanimid)	20.36	8.53	10.64	24.51			56	
Pentaerythritol ester of rosin, modified (Cellolyn 102, Hercules)	21.73	0.94	8.53	23.37			56	
Petroleum hydrocarbon resin (Piccopale 110, Penn. Ind. Chem.)	17.55	1.19	3.6	17.96			56	
Phenolic resin (resole, Phenodur 373U Chemische Werke Albert)	19.74	11.62	14.59	27.15			56	
Phenolic resin (Super Beckacite 1001, Reichhold)	23.26	6.56	8.35	25.57			56	
Poly(2-acrylamide-2-methyl propane sulphonamide) (tested in formamide/water mixtures)				43.6	Visc.	25	159	
Poly(3,3-dimethyl oxetane)	15.35	2.46	4.09	16.16	Visc.		92	
Poly(3,3-diethyl oxetane)	15.55	2.05	3.48	16.16	Visc.		92	
Poly(1,3-dioxolane)				20.66	Visc.	25	175	
Poly(ether urethane)				17.99 ± .02	IPGC	25	158	
Poly(DL-lactic acid)				17.38 ± 0.16	IPGC	100	158	
Poly(oxetane)	17.39	5.12	5.12	19.23	Obs.	21-24	110	
Poly(oxydimethylsilylene)				15.04	Swelling	76	110	
				14.9	Av.	76	110	
				15.45		118	110	
				15.6		45	110	
				14.9		125	110	
				15.59		145	110	
				15.4	Vapor sorp.	146	110	
				15	IPGC	146	110	
				15.1			110	

\* DGEBA – diglycidyl ether of bisphenol A; DDMe – tetraethyl derivative of DDM; DDM – diamino diphenyl methane; TGAP – triglycidyl derivative of amino phenol; ANI-aniline; DDS – diamino diphenylsulfone.

TABLE 10. cont'd

Polymer	Molar volume (cm <sup>3</sup> /gmol)	Solubility parameters (MPa) <sup>1/2</sup>				Method	T(°C)	Refs.
		δ <sub>d</sub>	δ <sub>p</sub>	δ <sub>h</sub>	δ			
$\delta_2 = (15.7 - 0.026)t$ , t in °C								
Poly(ethylene adipate)		16.3 ± 2	6.1 ± 0.5	9.4 ± 0.1	19.8 ± 2	IPGC	25	144
Poly(ethylene oxide)		17.3 ± 2	3.0 ± 1	9.4 ± 0.5	19.9 ± 2.2	IPGC	25	152
Poly(oxyethyleneoxyterephthaloyl)					17.8	Calc.	31	157
Poly(oxytrimethylene) polyoxetane -3,3 dimethyl -3,3 diethyl					19.64	IPGC	70	118
Poly(propylene oxide)					21.9	Visc.	25	112
					21.9	Visc.	25	157
Poly(sulfone), Bisphenol A (Udel)		19.03	0	6.96	20.26	Visc.	25	81
Poly(thioethylene)					19.23	Visc.	25	110
Poly(thiophenylethylene)					19.19	Visc.	25	43
Poly(urethane) (unknown composition)					18.4	Visc.	25	43
Poly(urethane), amorphous					19.0 ± 1.0	Visc.	25	87
Poly(vinyl ethylene)					20.5	Visc.	25	76
Poly(vinyl pyrrolidone)					20.5	Av.	25	76
Poly(vinyl methyl ketone)					22.9	Calc. <sup>HK</sup>	3	155
Poly(vinyl ethyl ketone)					22.92	Calc. <sup>HK</sup>	3	152
Poly(vinyl methyl sulfide)					22.14	Calc. <sup>HK</sup>	3	177
Poly(vinyl phenyl sulfide)					19.52	Calc. <sup>HK</sup>	3	177
Terpene resin (Piccolyte S-1000, Penn. Ind. Chem.)					20.28	Calc. <sup>HK</sup>	3	56
Urea-formaldehyde resin (Plastopal H, BASF)		16.47	0.37	2.84	16.72			56
Viton		20.81	8.29	12.71	25.74			130
		17	10.3	6.1	20.8			

<sup>a</sup>Altered from previously published value.

<sup>b</sup>Method of van Krevelen and Hoflyze.

<sup>c</sup>Method of Small.

<sup>d</sup>Method of Hoy.

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## Optically Active Polymers

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**A. Abbreviations used**

VII-715      4.4. Poly(styrenes) VII-735  
 VII-716      4.5. Poly(dienes) VII-735  
 VII-716      4.6. Poly(isonitriles) VII-736  
 VII-716      4.7. Poly(maleimides) VII-736  
 VII-717      4.8. Other Compounds VII-737

**B. Optically Active Polymers from Chiral Monomers**

VII-716      Table 5. Main-Chain Acyclic Heteroatom Polymers VII-737

**Table 1. Main-Chain Acyclic Carbon Polymers**

VII-716      5.1. Poly(oxides) and Poly(sulfides) VII-737

1.1. Poly(alkenes)

VII-716      5.2. Poly(isocyanates) VII-738

1.2. Poly(acrylics) and Related Polymers

VII-716      VII-739

1.3. Poly(methacrylics) and Related Polymers

1.4. Poly(vinyl ethers), Poly(vinyl ketones), and Poly(vinyl esters)

1.5. Poly(styrenes), Poly(carbazoles)

1.6. Poly(dienes)

1.7. Poly(isonitriles)

1.8. Poly(alkynes)

1.9. Poly(maleimides) and Related Polymers

1.10. Other Compounds

Table 2. Main-Chain Acyclic Heteroatom Polymers

2.1. Poly(oxides)

2.2. Poly(esters)

2.3. Poly(sulfides), Poly(thioesters)

2.4. Poly(urethanes), Poly(ureas)

2.5. Poly(amides)

2.6. Poly(isocyanates)

2.7. Poly(imines)

2.8. Poly(amino acids)

Table 3. Poly(saccharides)

C. Optically Active Polymers from Achiral Monomers

VII-733      VII-733

Table 4. Main-Chain Acyclic Carbon Polymers

4.1. Poly(acrylics) and Related Polymers

4.2. Poly(methacrylics) and Related Polymers

4.3. Poly(vinyl ethers)

VII-723      4.4. Poly(styrenes) VII-735  
 VII-723      4.5. Poly(dienes) VII-735  
 VII-723      4.6. Poly(isonitriles) VII-736  
 VII-723      4.7. Poly(maleimides) VII-736  
 VII-723      4.8. Other Compounds VII-737

VII-723      Table 5. Main-Chain Acyclic Heteroatom Polymers VII-737  
 VII-723      5.1. Poly(oxides) and Poly(sulfides) VII-737  
 VII-723      5.2. Poly(isocyanates) VII-738

D. References VII-739

By definition the optical activity,  $[M]_{\lambda}$ , of polymers and their low molecular weight analogs is given by

$$[M]_{\lambda} = [\alpha]_{\lambda} \times (\text{mean residue weight})/100$$

**A. ABBREVIATIONS USED**

AcAc	Acetylacetone
AIBN	Azobisisobutyronitrile
BPO	Benzoyl peroxide
DBP	Dibenzoyl peroxide
DCA	Dichloroacetic acid
DCM	Dichloromethane
DDB	2,3-Dimethoxy-1,4-bis(dimethylamino)butane
DMAc	Dimethylacetamide
DMF	Dimethylformamide
DMSO	Dimethylsulfoxide
DPEDA-Li	<i>N,N'</i> -diphenylethylenediamine monolithium amide
EDC	Ethylene dichloride
M	Monomer
MC	Model compound
NCA	<i>N</i> -Carboxylic anhydride
P	Polymer
RT	Room temperature
TMEDA	<i>N,N,N',N'</i> -tetramethylmethylenediamine
TCA	Trichloroacetic acid
TFA	Trifluoroacetic acid
TFEL	Trifluoroethanol
THF	Tetrahydrofuran