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Method for Estimating Solubility Parameter

The rapid method for estimation of solubility parameter which has recently been developed is of great value to laboratory workers because it reduces the amount of experimentation and computation required to obtain the cohesive density value or the solubility parameter of polymers. The solubility parameter is a measure of intermolecular forces; it is useful for assessment of material compatibility, glass-transition temperature, and transport properties.

Semiempirical correlations between solubility parameters and refractive indices for a series of model hydrocarbon compounds and organic polymers have been developed. The correlations are developed from theoretical considerations; initially, it is indicated that cohesive-energy density is numerically equal to the negative potential energy of one cubic centimeter of the material (—E/V), where V is the molar volume and E is the potential energy of a mole of material. Then, the solubility parameter, δ, is defined as the square root of the cohesive-energy density, and it is noted that its value can be obtained from the heat of vaporization and the molar volume. Since the heat of vaporization for a polymer cannot be obtained directly, there is invoked Walden's empirical relationship for obtaining latent heat of vaporization from refractive index; after dropping minor terms, the resulting equation for solubility parameter is found to be:

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

where n is the refractive index and C is a constant which was found to have an average of 305 for fifty seven model compounds. However, the value of C varies significantly for different chemical types, and it is necessary to use the appropriate value of C (as determined by chemical structure) in order to obtain satisfactory values of solubility parameters. Following are C-values for a variety of polymers: poly(ethylene), 254.1; poly(isobutylene), 230.9; natural rubber, 230.9; poly(styrene), 287.6; poly(methyl acrylate), 304.5; poly (ethyl acrylate), 304.5; poly(propyl acrylate), 304.5; poly(butyl acrylate), 304.5; poly(vinylidene chloride), 330.8; poly(tetrafluoroethylene), 205.1; nitroso rubber, 205.1. C-values for different chemical types are: normal aliphatic hydrocarbons, 254.1 ±2.1; branched aliphatic hydrocarbons, 230.9 ±9.3; aliphatic ethers, 279.2 ±25.0; aliphatic esters, 353.3 ±30.9; normal aliphatic fluorocarbons, 205.1 ±9.5; chlorocarbons, 330.8 ±53.1; aromatics, 287.6 ±10.4.

Note:

Requests for further information may be directed to:

Technology Utilization Officer
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NASA has decided not to apply for a patent.

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