Table IV. Experimental Data for Ethyl Acetate (A)–Water (B) System Taken from Smith-Bonner Still at 760 Mm of Hg

Temp., °C	Ethyl Acetate, Mole Fraction		Temp., °C	Ethyl Acetate, Mole Fraction	
	Liquid	Vapor		Liquid	Vapor
91.0	...	0.297	73.0	0.908	0.765
83.7	...	0.459	73.5	0.934	0.791
70.9	0.124	0.693	73.6	0.934	0.788
70.9	0.385	0.688	73.7	0.939	0.787
70.9	0.548	0.710	74.4	0.974	0.876
71.9	0.851	0.724	75.4	0.978	0.911
72.6	0.894	0.757	75.9	0.986	0.917

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Terephthalic Acid Solubility

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The solubility of terephthalic acid was determined in toluene, anisole, 3-pentanone, and 1,4-dioxane. It correlates with the Brønsted basicity of the solvents previously correlated by an infrared spectral shift technique.

TEREPHTHALIC acid, which finds extensive use in poly(ethylene terephthalate) films and fibers, is one of the most intractable organic compounds *(10)*. Its high melting point [triple point, 427° C *(10)*] is consistent with its low solubility *(1, 2, 10)* in nonbasic solvents. Since most organic reactions are carried out in solution, the ability to predict the solubility of terephthalic acid would be very useful. We have determined its solubility in several organic solvents, and report a scheme which allows the solubility to be estimated.

EXPERIMENTAL

The terephthalic acid was 99.98% pure. The chief impurity was toluic acid (140 ppm). The solvents were reagent grade.

The solubilities were determined by weighing the terephthalic acid and solvent into a glass tube, which was sealed and submerged in a constant temperature bath thermostated to ±0.05° C. The bath temperature was raised 1° C per 10 minutes and the tube was shaken until all the acid was dissolved *(5, 11)*.

RESULTS AND DISCUSSION

The solubilities of terephthalic acid in toulene, anisole, 3-pentanone, 1,4-dioxane, and *N,N*-dimethylformamide are given in Table I. When the log of the mole fraction of terephthalic acid is plotted against the reciprocal of the temperature, a straight line is obtained for each solvent *(4)*, with correlation coefficients of 0.98 or better. Thus, the solubilities at other temperatures may be reliably obtained by extrapolation.

The solubility of some organic acids has been correlated with the dielectric constant of the solvent *(6)*, but no such correlation exists for terephthalic acid. Dioxane and toluene have similar dielectric constants *(9)*, but differ greatly in their ability to dissolve terephthalic acid.

Since terephthalic acid dissolves readily in basic media, it seemed possible that its solubility in any solvent might correlate with the Brønsted basicity—i.e., the proton-accepting ability of the solvent. Recently this property was correlated for a number of organic solvents at 25° *(3, 7)* by measuring the shift, $\Delta\nu$, of the infrared stretching frequency of methanol-*D* in a given solvent from its position in benzene.

Table I. Terephthalic Acid Solubility

Solvent	Grams of Acid/100 Grams of Solvent	Mole Fraction	Temp., °C	Correlation Coefficient[a]
Toluene	0.0779	0.000431	227	−0.98
	0.0577	0.000319	221	
	0.0415	0.000230	212	
Anisole	0.410	0.0268	245.5	−1.00
	0.345	0.0225	240	
	0.145	0.00947	215	
3-Pentanone	0.335	0.0212	185.5	−1.00
	0.280	0.0178	175	
	0.145	0.00919	144	
1,4-Dioxane	1.824	0.0131	198.5	−1.00
	0.928	0.00672	160.5	
	0.464	0.00337	124	
N,N-Dimethyl-formamide[b]	7.4	0.0315	25	

[a] Correlation coefficient for plot of log mole fraction of terephthalic acid against reciprocal of temperature. [b] *(8)*.

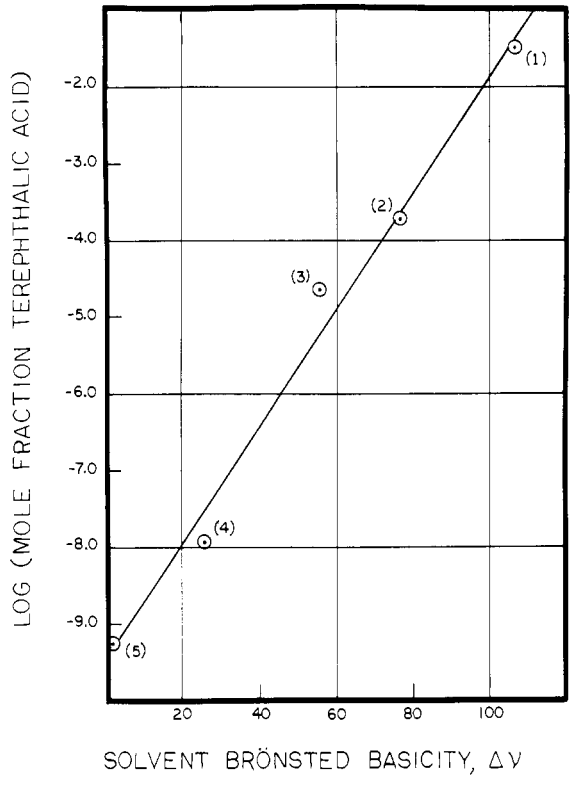

Figure 1. Terephthalic acid solubility and solvent basicity at 25° C

1. *N,N*-Dimethylformamide
2. 1,4-Dioxane
3. 3-Pentonone
4. Anisole
5. Toluene

Table II. Correlation of Terephthalic Acid Solubility and Brønsted Basicity of Solvent at 25° C

Solvent	Mole Fraction Terephthalic Acid[a]	Brønsted Basicity, $\Delta\nu$[b]
Toluene	5.50×10^{-10}	2
Anisole	1.19×10^{-8}	26
3-Pentanone	2.24×10^{-5}	56
1,4-Dioxane	1.93×10^{-4}	77
N,N-Dimethylformamide	3.15×10^{-2}	107

[a] Experimental for *N,N*-dimethylformamide, extrapolated for other solvents. [b] *(6)*.

The values of log (terephthalic acid solubility at 25°), either experimental or extrapolated, and the values of $\Delta\nu$ for our five solvents are listed in Table II and plotted in Figure 1. The equation for the straight line is

$$\log \chi = 0.0759\,\nu - 9.478$$

where χ is the mole fraction of terephthalic acid. The correlation coefficient for this line is 0.99. Evidently the solubility of terephthalic acid can be estimated for any solvent for which $\Delta\nu$ has been determined.

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