# Solubility Parameters of Polymethacrylonitrile, Poly(Methacrylic Acid) and Methacrylonitrile/ Methacrylic Acid Copolymer

#### BANG-CHEIN HO, WEI-KUO CHIN, and YU-DER LEE\*

Department of Chemical Engineering, National Tsing Hua University, Hsiuchu, Taiwan, Republic of China 30043

### **SYNOPSIS**

The solubility behaviors of polymethyacrylonitrile (PMAN), poly(methacrylic acid) (PMAA), and its random copolymer methacrylonitrile (MAN)/methacrylic acid (MAA) in various solvents were investigated. The results were used in a computer program to obtain a 3-dimensional representation of the polymer solubility region in the Hansen space. Thus, the values of dispersion  $(\delta_{d,p})$ , polar  $(\delta_{p,p})$  and hydrogen bonding  $(\delta_{h,p})$  components of the total solubility parameter  $(\delta_{t,p})$  were obtained. Comparisons between the experimental results and the estimated values are discussed. Also, prediction for solubility parameter values for MAN/MAA copolymer via their homopolymers, PMAN, and PMAA has been evaluated.

# INTRODUCTION

Homopolymers, polymethacrylonitrile (PMAN) and poly(methacrylic acid) (PMAA), and random copolymers poly(MAN-co-MAA) have been studied frequently due to their potential uses as photoresist materials. However, most efforts had been devoted to the properties of thermal degradation.<sup>1-7</sup> Very little information is available on their solubility behavior in solvents.

On the predication of total solubility parameter, the following equation is often used

$$\delta_t = \left(\frac{E_{\rm coh}}{V}\right)^{1/2} \tag{1}$$

where  $E_{\rm coh}$  is the cohesive energy and V is the molar volume. Dunkle<sup>8</sup> derived group contributions for the cohesive energy of liquids at room temperature. Hayes,<sup>9</sup> Di Benedetto,<sup>10</sup> Hoftyzer and Van Krevelen<sup>11</sup> have applied Dunkel's method to polymers. Small<sup>13</sup> has demonstrated that the combination  $(E_{\rm coh}V(298 \text{ K}))^{1/2} = F$ , the molar attraction constant, is a useful additive quantity for low-molecular as well as for high-molecular substances. Hoy<sup>14</sup> and Van Krevelen<sup>15</sup> also derived a set of group contributions and atomic contributions to calculate F. Therefore, the value of  $E_{\rm coh}$  for polymer can be calculated from F also.

For many liquids and amorphous polymers, the cohesive energy is also dependent on the interaction between polar groups and on hydrogen bonding. Therefore, the cohesive energy may be divided into three parts, corresponding to the three types of interaction forces:

$$E_{\rm coh} = E_d + E_p + E_h$$

where  $E_d$ ,  $E_p$ , and  $E_h$  are contributions of dispersion, polar, and hydrogen bonding forces, respectively. The corresponding equation for the total solubility parameter ( $\delta_t$ ) is

$$\delta_t^2 = \delta_d^2 + \delta_p^2 + \delta_h^2 \tag{2}$$

where  $\delta_d$ ,  $\delta_p$ , and  $\delta_h$  are the solubility parameters due to dispersion, polar, and hydrogen bonding forces. Unfortunately, values of  $\delta_d$ ,  $\delta_p$ , and  $\delta_h$  cannot be determined directly.

<sup>\*</sup> To whom all correspondence should be addressed. Journal of Applied Polymer Science, Vol. 42, 99–106 (1991)

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Hansen<sup>16-18</sup> treated the solubility parameter as a vector in a three-dimensional  $\delta_d$ ,  $\delta_p$ ,  $\delta_h$  space. From the experimental measurements of the solubility parameter of a number polymers in a series of solvents, theoretical calculations, and plenty of computer fitting, the individual components  $\delta_d$ ,  $\delta_p$ , and  $\delta_h$  of many solvents and polymers have been developed and tabulated.<sup>19,20</sup>

In this paper, the solubility behavior of homopolymer, PMAN and PMAA, and MAN/MAA copolymer in 55 solvents with known solubility parameters has been examined. From these experiments the solubility regions of the homopolymers and copolymer in 3-dimensional Hansen space<sup>16-18</sup> have been determined and the values of solubility parameters evaluated. The total solubility parameters as well as their components for these polymers were also calculated from the group contribution method.<sup>19,20</sup> Comparisons between the experimental results and the calculated values are also discussed.

# **EXPERIMENTAL**

#### Materials

Methacrylonitrile (MAN) was washed with saturated aqueous sodium hydrogen sulfite (NaHSO<sub>3</sub>) first, then with 1 wt % sodium hydroxide (NaOH) in saturated aqueous sodium chloride (NaCl) followed by saturated aqueous NaCl. The MAN was dried with calcium chloride (CaCl<sub>2</sub>) and fractionally distilled under nitrogen in order to separate it from impurities. Methacrylic acid (MAA) was distilled under reduced pressure before use.  $\alpha, \alpha'$ -Azobisisobutyrontrile (AIBN) was recrystallized from methanol, and dried under reduced pressure at 25°C. Both homopolymers, PMAN and PMAA, were obtained from Polysciences, Inc. without further purification. All liquids used for solubility experiments were of reagent grade and used without further purification.

## Copolymerization

The polymerization of MAN/MAA copolymer was performed in bulk, using AIBN as a free radical initiator. A solution prepared from 1.286 mol of MAN and 0.714 mol of MAA were placed in 1-L, threeneck, round-bottom flask equipped with a stirring mechanism, reflux condensor, and nitrogen gas inlet. The mixture of monomer was then heated to  $65^{\circ}$ C in the presence of following N<sub>2</sub> gas. A free-radical initiator consisting of 0.25 wt % to monomer of AIBN was added to initiate the polymerization. The polymerization was carried out at 65°C for 2 h. After polymerization, the polymer was precipitated with water and reprecipitated from dimethyl formamide (DMF) solution. It was ground to a fine powder and dried in a vacuum oven at 50°C for 24 h. The composition of the MAN/MAA copolymer was determined by elemental analysis, the molar fraction of MAN was found to be  $X_{MAN} = 0.525$ . The intrinsic viscosity of the MAN/MAA copolymer was measured at 30°C in DMF solution using a Ubbelohde viscometer and was found to be  $4.18 \, dL/g$ . The density of the MAN/MAA copolymer measured at 25°C using a volume-calibrated pycnometer was 1.16 g/ cm<sup>3</sup> while those of the homopolymers, PMAN and PMAA, were 1.04 and 1.29 g/cm<sup>3</sup>, respectively.

# **Film Preparation**

To better evaluate the solubility behavior of the polymers in testing liquids, powder from the polymers were transformed into films by following procedure. A concentrated solution (10-20 wt % polymer) mer in dimethyl sulfoxide) was first cast at room temperature on a cleaned glass plate, and placed in a force-ventilation oven at 75°C for 8 h to evaporate the solvent. Then to allow complete solvent evaporation, dried under vacuum at 75°C for 24 h. After cooling at room temperature, the corresponding film was leached with water (homopolymer PMAA was leached with acetone) overnight in a Soxhlet apparatus, vacuum dried, and finally cut into strips for solubility tests.

# **Solubility Tests**

Solubility tests were carried out by the following procedures.<sup>16–18</sup> Strips of  $0.2000 \pm 0.0005$  g were immersed in 2 mL of liquid in sealed glass tubes. The tubes were placed in a water bath at 25°C and continuously shaken for 7 days. After 7 days, the samples were inspected. Since the dissolving rate of polymers in some solvents was extremely low at room temperature, in some cases samples were heated to 70°C, for the same time interval afterwards they were cooled to 25°C for visual inspection. On the basis of their ability to dissolve or swell the polymer, the liquids were classified into four categories: good solvent, good swelling agent, poor swelling agent, and nonsolvent. Table I lists the liquids used and their extents of solubilities for PMAN, PMAA, and poly(MAN-co-MAA).

No.         Liquid         b <sub>a</sub> b <sub>a</sub> b <sub>b</sub> PMAN         Copolym.         PMAA           1         Acetic andydride         7.1         3.9         6.6         10.5         4         3         3           2         Acetic andydride         7.8         5.7         6.0         10.9         1         1         3           3         Acetonitrile         7.5         8.8         3.0         11.9         1         4         4           6         Antilne         9.5         2.5         4.9         11.0         1         4         4           6         Antilne         9.5         2.5         4.9         11.0         1         4         4           7         Benzalebyde         9.2         4.2         2.6         10.4         1         4         4           9         Benzyl actate         7.7         1.8         2.8         7.7         1.1.3         4         4         4           12         Chorobenzene         9.3         2.1         1.0         8.4         4         4         4           14         Chorobenzene         8.7         1.5         2.8         9.3							E	Extent of Solubilit	у
1Acetic ank Acetic ankylinide7.13.96.610.54332Acetic ankylinide7.85.75.010.91133Acetonirrile7.65.13.49.81.234Acetonirrile7.58.83.011.91445Acrylonirlile8.08.53.312.11446Anilize9.52.54.911.01447Benzele9.00.51.09.04448Benzele9.00.51.09.0444101-Butanol7.82.87.711.344412Chlorobenzene9.32.11.09.644413t-Chlorbutane7.53.41.78.44414Chlorobenzene8.32.11.09.644414Chlorobenzene8.73.12.59.334414Chlorobenzene8.73.12.59.614415m-Cresol8.20.00.08.244416m-Cresol8.20.00.08.244417Cyclobezance8.73.12.59.6144181.2 </th <th>No.</th> <th>Liquid</th> <th><math>\delta_{d,s}</math></th> <th><math>\delta_{p,s}</math></th> <th><math>\delta_{h,s}</math></th> <th><math>\delta_{t,s}</math></th> <th>PMAN</th> <th>Copolym.</th> <th>PMAA</th>	No.	Liquid	$\delta_{d,s}$	$\delta_{p,s}$	$\delta_{h,s}$	$\delta_{t,s}$	PMAN	Copolym.	PMAA
2Acetic anlydride7.85.75.01.91133Acetome7.65.13.49.81.11444Acetomitrile7.58.83.011.91446Aniline9.52.54.911.01447Benzene9.00.51.09.04448Benzene9.00.51.09.04449Benyi lachol7.82.87.711.3444101-Butanol7.82.87.711.344411n-Buty acetate7.71.88.18.544412Chloroberzne7.53.41.18.4444131-Chloroberane8.71.52.89.334414Cyclohezano8.20.008.24.444415mrCresol8.73.12.59.6344416Cyclohezano8.73.12.59.6344417Cyclohezano8.82.56.51.1111121810.101.41.81.01.4112119Dieblyristeine7.81.88.08.01.301 <td< td=""><td>1</td><td>Acetic acid</td><td>7.1</td><td>3.9</td><td>6.6</td><td>10.5</td><td>4</td><td>3</td><td>3</td></td<>	1	Acetic acid	7.1	3.9	6.6	10.5	4	3	3
3Acetone7.68.18.49.81234Acrylonitrile8.08.53.311.91445Acrylonitrile8.08.53.312.11446Anilne9.24.22.610.41447Benzaldehyde9.24.22.610.41449Benzyl alcohol9.00.51.09.09.04449Benzyl alcohol9.03.16.711.722411n-Butyl acetate7.71.83.18.644412Chloroberzane9.32.11.09.64441314.1141.78.444414Chloroberane8.71.52.89.334415m.Cresol8.82.66.311.114416Cyclohezane8.20.00.08.244417Cyclohezane8.20.00.08.2444181.2-Dichlorothane6.95.54.59.6111114142.57.7444410Diethyl alkohr7.81.82.01.311114142.5<	2	Acetic anhydride	7.8	5.7	5.0	10.9	1	1	3
4Acetonitrile7.58.83.01.91446Aniline9.52.53.412.11446Aniline9.52.54.911.01447Benzene9.00.51.09.04448Benzene9.00.51.09.0444101-Butanol7.82.87.711.344411n-Butyla ectate7.71.88.18.544412Chlorobenzene9.32.11.09.6444131.Chorubane8.71.52.89.3344414Chlorobenzene8.71.52.89.8344415m-Cresol8.71.12.59.6144416Cyclohezano8.73.12.59.6144417Cyclohezano7.81.82.08.3444418Disbutyl storne7.81.82.08.3444421Disbutyl storne7.81.82.08.3444422N/N-dimethyl acetanide8.56.75.512.1111224Minethyl acetanide8.56.7 <td>3</td> <td>Acetone</td> <td>7.6</td> <td>5.1</td> <td>3.4</td> <td>9.8</td> <td>1</td> <td>2</td> <td>3</td>	3	Acetone	7.6	5.1	3.4	9.8	1	2	3
5Acrylonitrile8.08.53.312.11447Benzaldehyde9.52.54.011.01447Benzalchyde9.24.22.610.41448Benzyl alcohol9.00.16.711.72249Benzyl alcohol9.00.16.711.722411n-Butyl actate7.71.83.18.544412Chlorobenzene9.32.11.09.6444131.Chlorbutane7.53.41.78.444414Chloroform8.71.52.89.3344415m.Cresol8.73.12.69.6344416Cyclobexance8.20.00.08.244410Diethlene glycol7.97.210.01.4.641112Diebhexalone7.81.82.01.3.0111224Diethlene glycol7.97.210.01.4.64444251.5.65.011.111221.4.2111224Diethlene glycol7.94.57.011.54222333<	4	Acetonitrile	7.5	8.8	3.0	11.9	1	4	4
6Aniline9.52.54.91.101448Benzene9.00.51.09.01448Benzene9.00.51.09.03.16.711.7224101-Butanol7.82.87.711.34444111-Chlorobenzene9.32.11.09.6444412Chlorobenzene7.71.83.11.78.44444131-Chlorobtane7.53.41.78.44444414Chloroform8.71.52.89.33444 <td>5</td> <td>Acrylonitrile</td> <td>8.0</td> <td>8.5</td> <td>3.3</td> <td>12.1</td> <td>1</td> <td>4</td> <td>4</td>	5	Acrylonitrile	8.0	8.5	3.3	12.1	1	4	4
7Bernzaldehyde9.24.22.610.41449Bernzyl alcohal9.00.11.09.01.17.1.72249Bernzyl alcohal9.00.16.711.7224411n-Butyl acetate7.71.83.18.5444412Chlorobernzene9.32.11.09.64444131.Chlorbutane9.71.52.89.3344414Chloroform8.71.52.89.3344415m-Cresol8.82.56.311.11444416Cycloberano8.73.12.59.63444417Cycloberano8.73.12.59.634444181.2-Dichloroethane6.95.54.59.63444420Diethlene glycol7.97.210.014.64111221N-M-dimethyl alcetanide8.25.65.011.1112222N/N-dimethyl alcetanide8.25.65.013.033333231.4-Dioxane9.08.610.033333 <t< td=""><td>6</td><td>Aniline</td><td>9.5</td><td>2.5</td><td>4.9</td><td>11.0</td><td>1</td><td>4</td><td>4</td></t<>	6	Aniline	9.5	2.5	4.9	11.0	1	4	4
8Benzene9.00.51.09.04.1444101-Butanol7.82.87.711.344411n-Butyl acetate7.71.83.18.544412Chlorobenzene9.32.11.09.6444131-Chlorbutane7.53.41.78.444414Chlorobenzene8.71.52.89.3344415 <i>m</i> -Cresol8.82.56.311.1144416Cyclohezano8.73.12.59.61444417Cyclohezano8.73.12.59.61444	7	Benzaldehyde	9.2	4.2	2.6	10.4	1	4	4
9Benzyl alcohol9.03.16.711.7224101. Butanol7.82.87.71.83.18.544411n-Butyl actate7.71.83.18.544412Chlorobenzene9.32.11.09.6444131-Chlorbutane7.53.41.78.444414Chloroform8.71.52.89.3344415m-Cresol8.82.56.31.1144416Cyclohexance8.73.12.59.61444181.2-Dichloreothane6.95.54.59.6344420Diethlene glycol7.97.210.01.4.6411210Diethlene glycol7.97.210.01.4.6411222N.N-dimethyl alcetamide8.25.65.01.1.1112223N.N-dimethyl alcetamide9.08.010.0333324Dimethyl sloride9.08.610.03333251.4.10xane9.08.610.0333326HAnol7.77.01.5.58.84444 <td>8</td> <td>Benzene</td> <td>9.0</td> <td>0.5</td> <td>1.0</td> <td>9.0</td> <td>4</td> <td>4</td> <td>4</td>	8	Benzene	9.0	0.5	1.0	9.0	4	4	4
10       1-Butanol       7.8       2.8       7.7       11.3       4       4       4         11       n-Butyl acetate       7.7       1.8       3.1       8.5       4       4         12       Chloroberszee       9.3       2.1       1.0       9.6       4       4         13       1-Chlorobrane       7.5       3.4       1.7       8.4       4       4         14       Chloroberszee       8.7       3.1       2.5       6.3       11.1       1       4       4         15       m-Cresol       8.8       2.5       6.3       11.1       1       4       4         16       Cyclohexano       8.7       3.1       2.5       9.6       3       4       4         17       Okichlene glycol       7.9       3.1       2.5       9.6       3       4       4         18       1.2.0chloroethane       6.9       5.5       4.5       9.6       3       4       4         21       Dinebutyl settene       7.8       1.8       2.0       8.3       4       4       4         22       N/A-dimethyl acetamide       8.6       6.7       5.5 <t< td=""><td>9</td><td>Benzyl alcohol</td><td>9.0</td><td>3.1</td><td>6.7</td><td>11.7</td><td>2</td><td>2</td><td>4</td></t<>	9	Benzyl alcohol	9.0	3.1	6.7	11.7	2	2	4
11 $n$ -Butyl actata7.71.83.18.544412Chorobenzene3.32.11.09.6444131-Chlorobutane7.53.41.78.444414Choroform8.73.52.89.3344415 $m$ -Cresol8.82.56.31.1.1144416Cyclohexance8.73.12.59.6144417Cyclohexance8.73.12.59.61444181.2-Dichloroethane6.95.54.59.6144420Diethlene glycol7.97.210.014.6411221Dinethyl actamide8.25.65.011.1112223N/A-dimethyl formamide8.55.65.013.011111224Dimethyl suffoxide9.08.05.013.0334	10	1-Butanol	7.8	2.8	7.7	11.3	4	4	3
12Chlorobenzene9.32.11.09.6444131-Chlorobram7.53.41.78.44414Chloroform8.71.52.89.334415 $m$ -Cresol8.82.56.311.114416Cyclohexano8.20.00.08.244417Cyclohexanone8.73.12.59.6144181.21.20.6144419Diethyl ether7.11.42.57.744421Diisobutyl ketone7.81.82.08.344422N.N-dimethyl actamide8.25.65.011.1112123M.N-dimethyl formamide8.30.93.610.01112124Dimethyl aufoxide9.08.05.013.01112125Ethanol7.72.63.58.8444426Ethanol7.72.63.58.844427Ethyl actata7.72.63.58.844428Ethyl actata7.72.63.58.844430Ethyl actata7.62.21.1.54222 <td>11</td> <td>n-Butyl acetate</td> <td>7.7</td> <td>1.8</td> <td>3.1</td> <td>8.5</td> <td>4</td> <td>4</td> <td>4</td>	11	n-Butyl acetate	7.7	1.8	3.1	8.5	4	4	4
131-Chlorbutane7.53.41.78.444414McDroform8.71.52.89.334415m-Cresol8.82.56.311.114416Cyclohexane8.20.00.08.244417Cyclohexane6.95.54.59.6344181.2-Dichlorothane6.95.54.59.634420Diethlene glycol7.97.210.014.6411221Disobutyl etone7.81.82.08.3444422N.N-dimethyl acetamide8.25.65.011.1112223N.N-dimethyl acetamide8.25.65.013.01111224Dimethyl suffxide9.08.05.013.011112251.4-Dioxane9.30.93.610.0321122261.4-Dioxane7.72.63.58.844444292.Ethyl hexanol7.81.65.89.9444430Ethyl acetate7.72.63.58.8444431Formic acid7.05.88.1 <td< td=""><td>12</td><td>Chlorobenzene</td><td>9.3</td><td>2.1</td><td>1.0</td><td>9.6</td><td>4</td><td>4</td><td>4</td></td<>	12	Chlorobenzene	9.3	2.1	1.0	9.6	4	4	4
14Chloroform $87$ $1.5$ $2.8$ $9.3$ $3$ $4$ $4$ 15 $m$ -Cresol $8.8$ $2.5$ $6.3$ $11.1$ $1$ $4$ $41$ 16Cyclohexano $8.7$ $3.1$ $2.5$ $9.6$ $1$ $4$ $41$ 17Cyclohexano $6.9$ $5.5$ $4.5$ $9.6$ $3$ $4$ $44$ 181.2Dischyl ether $7.1$ $1.4$ $2.5$ $7.7$ $4$ $4$ $44$ 20Dischyl ether $7.8$ $1.8$ $2.0$ $8.3$ $4$ $4$ $41$ 21Dissobutyl ketone $7.8$ $1.8$ $2.0$ $8.3$ $4$ $4$ $41$ 22 $N.N$ -dimethyl formamide $8.2$ $5.6$ $5.0$ $11.1$ $1$ $1$ $21$ 23 $N.N$ -dimethyl formamide $8.2$ $5.6$ $5.0$ $13.0$ $1$ $1$ $1$ $21$ 24Dimethyl sulfoxide $9.0$ $8.0$ $5.0$ $13.0$ $3$ $2$ $11$ $21$ 25Ethanol $7.7$ $4.3$ $9.5$ $13.0$ $3$ $2$ $11$ $21$ 26Ethanol $7.7$ $2.6$ $5.8$ $8.1$ $12.2$ $1$ $2$ $23$ 27Ethanol $7.2$ $0.0$ $0.0$ $7.2$ $4$ $4$ $41$ 29 $2$ -Ethyl hexanol $7.8$ $1.6$ $5.8$ $9.9$ $4$ $4$ $41$ 29 $2$ -Ethyl hexanol $7.8$ $4.6$ <td< td=""><td>13</td><td>1-Chlorbutane</td><td>7.5</td><td>3.4</td><td>1.7</td><td>8.4</td><td>4</td><td>4</td><td>4</td></td<>	13	1-Chlorbutane	7.5	3.4	1.7	8.4	4	4	4
15m-Cresol8.82.56.311.114416Cyclohexanone8.20.00.08.24417Cyclohexanone8.73.12.59.6144181.2-Dichlorethane6.95.54.59.6344181.2-Dichlorethane7.11.44.257.744420Diethlene glycol7.97.210.014.64111221N.N-dimethyl acetamide8.25.65.011.1112223N.N-dimethyl acetamide8.06.75.512.1111224Dimethyl suffoxide9.08.05.013.03211251.4-Dioxane9.30.93.610.03333326Ethanol7.74.63.68.810.03321227Ethanol anine7.72.63.58.812.212328M-Heytaenol7.81.65.89.9444292.Ethyl hexanol7.81.65.89.944430Ethanolenoire7.84.16.11.044431A4444444 <tr< td=""><td>14</td><td>Chloroform</td><td>8.7</td><td>1.5</td><td>2.8</td><td>9.3</td><td>3</td><td>4</td><td>4</td></tr<>	14	Chloroform	8.7	1.5	2.8	9.3	3	4	4
16Cyclohexane8.20.00.08.244417Cyclohexane8.73.12.59.6144181.2.Dichloreethane6.95.54.59.634419Diethyl ether7.11.42.57.744410Disobutyl ketone7.81.82.08.344421Disobutyl ketone7.81.82.08.344422N.N-dimethyl ormamide8.56.75.51.1.111224Dimethyl sulfoxide9.08.05.013.01111224Dimethyl sulfoxide9.08.05.013.032112251.4 - Dixane9.30.93.610.033 <td< td=""><td>15</td><td>m-Cresol</td><td>8.8</td><td>2.5</td><td>6.3</td><td>11.1</td><td>1</td><td>4</td><td>4</td></td<>	15	m-Cresol	8.8	2.5	6.3	11.1	1	4	4
17 $Cyclohesnone$ 8.73.12.59.6144181.2-Dichloroethane6.95.54.59.634419Diethlee glycol7.97.210.014.641120Diethlee glycol7.97.210.014.641121Disobutyl ketone7.81.82.08.344422N/N-dimethyl acetamide8.25.65.011.111223N/N-dimethyl formamide8.56.75.512.1111224Dimethyl sulfoxide9.08.05.013.011112251.4-Dioxane9.30.93.610.033	16	Cyclohexane	8.2	0.0	0.0	8.2	4	4	4
181.2-Dichlorosthane6.95.54.59.634419Diethlene glycol7.97.210.014.641121Disobutyl ketone7.81.82.08.344421N.V-dimethyl cetamide8.25.65.011.111223N.V-dimethyl cetamide8.56.75.512.1111224Dimethyl sulfoxide9.08.05.013.01111224Dimethyl sulfoxide9.08.010.0333<	17	Cyclohexanone	8.7	3.1	2.5	9.6	1	4	4
19Diethyl ether7.11.42.57.744420Diethlene glycol7.97.210.014.641121Disobutyl ketone7.81.82.08.344422N.N-dimethyl acetamide8.25.65.011.111224Dimethyl solfoxide9.08.05.013.01111251.4-Dioxane9.30.93.610.0332126Ethanol7.74.39.513.0321127Ethanol amine8.47.610.415.4112228Ethyl acetate7.72.63.58.8444430Ethyl cellocolve7.94.57.011.5422232n-Heytane7.20.00.07.2444433n-Hexanethyl phosphoramide9.04.25.511.31444441510.04444444433n-Heytanethyl phosphoramide9.04.25.511.3144434Norbenzene7.84.42.59.3244435Isopropyl ether6.72.30.77.0	18	1,2-Dichloroethane	6.9	5.5	4.5	9.6	3	4	4
20Diethlene glycol7.97.210.014.641121Diisobutyl ketone7.81.82.08.344422N.N-dimethyl cetamide8.56.75.512.111223N.N-dimethyl cornamide8.56.75.512.1111224Dimethyl sulfoxide9.08.05.013.01111251.4-Dioxare9.30.93.610.033326Ethanol7.74.39.513.032127Ethanol amine8.47.610.415.411228Ethyl acetate7.72.63.58.8444292-Ethyl hexanol7.81.65.89.9444292-Ethyl cellocolve7.94.57.011.542231Formic acid7.05.88.112.212332 <i>n</i> -Heytane7.20.00.07.244434Iscamyl alcohol6.84.16.110.044435Isoropyl ether6.73.53.77.134436Methyl acetate7.63.53.77.134439Methyl acetate7.84.4	19	Diethyl ether	7.1	1.4	2.5	7.7	4	4	4
21Disobutyl ketone7.81.82.08.344422 $N_i$ N-dimethyl acetamide8.25.65.011.111223 $N_i$ N-dimethyl formamide8.56.75.512.1111224Dimethyl sulfoxide9.08.05.013.01111251.4-Dioxane9.30.93.610.0333326Ethanol7.74.39.513.0321127Ethanol amine8.47.610.415.411228Ethyl acetate7.72.63.58.844430Ethyl cellocolve7.94.57.011.5422231Formic acid7.05.88.112.21233337n-Heytane7.20.00.77.0444438n-Heytane7.63.53.79.1344434Isopropyl ether6.72.30.77.044436Methyl exophene7.84.42.511.314437Methyl etohyl ktone7.84.22.010.914438N-methyl-2-pyrolidone8.86.03.511.211	20	Diethlene glycol	7.9	7.2	10.0	14.6	4	1	1
22N,N-dimethyl acetamide8.25.65.011.111223N,N-dimethyl formamide8.56.75.512.1111224Dimethyl sulfoxide9.08.05.013.011112251,4-Dioxane9.30.93.610.0333326Ethanol7.74.39.513.0321127Ethanol amine8.47.610.415.4112228Ethyl acetate7.72.63.58.84444292.Ethyl hexanol7.81.65.89.9444430Ethyl cellocolve7.94.57.011.5422231Formic acid7.05.88.112.2123332 <i>n</i> -Heptane7.20.00.07.244434Isoamyl alcohol6.84.16.110.044435Isoamyl alcohol6.84.16.110.044436Methyl acetate7.63.53.79.134437Methyl acetate7.84.42.59.324438Methyl acetate7.87.62.211.114 </td <td>21</td> <td>Diisobutyl ketone</td> <td>7.8</td> <td>1.8</td> <td>2.0</td> <td>8.3</td> <td>4</td> <td>4</td> <td>4</td>	21	Diisobutyl ketone	7.8	1.8	2.0	8.3	4	4	4
23N,N-dimethyl formamide8.56.75.512.1111224Dimethyl sulfoxide9.08.05.013.01111251,4-Dioxane9.30.93.610.033326Ethanol7.74.39.513.032127Ethanol amine8.47.610.415.411228Ethyl acetate7.72.63.58.8444292-Ethyl hexanol7.81.65.89.944430Ethyl acetate7.05.88.112.212332n-Heptane7.20.00.07.244443n-Hexamethyl phosphoramide9.04.25.511.31444415Isopropyl ether6.72.30.77.044436Methyl acetate7.63.53.79.134447Methyl ethyl ketone7.84.22.010.914439Methyl ethyl ketone7.87.62.211.114448N-methyl-2-pyrolidone8.86.03.511.211339Methyl ethyl ketone7.87.62.211.114441Nitrobenz	22	N.N-dimethyl acetamide	8.2	5.6	5.0	11.1	1	1	2
24Dimethyl sulfoxide9.08.05.01.11111251,4-Dioxane9.30.93.610.033326Ethanol7.74.39.513.032127Ethanol amine8.47.610.415.411228Ethyl actate7.72.63.58.8444292-Ethyl hexanol7.81.65.89.944420Ethyl cellocolve7.94.57.011.5422231Formic acid7.05.88.112.212332n-Hexamethyl phosphoramide9.04.25.511.314434Isoamyl alcohol6.84.16.110.044435Isopropyl ether6.72.30.77.044436Methyl actate7.63.53.79.134437Methyle ktone7.84.42.59.324438N-methyl-2-pyrolidone8.86.03.511.211339Methyle acthare7.87.62.211.114441Nitrobenzene9.88.22.010.914442Nitrobenzene9.88.8<	23	N.N-dimethyl formamide	8.5	67	5.5	12.1	1	1	2
1.4 - Dioxane0.30.30.40.01111251.4 - Dioxane9.30.93.610.033326Ethanol7.74.39.513.032127Ethanol amine8.47.610.415.411228Ethyl acetate7.72.63.58.8444292-Ethyl hexanol7.81.65.89.944430Ethyl cellocolve7.94.57.011.542231Formic acid7.05.88.112.212332n-Heptane7.20.00.07.244443Isoamyl alcohol6.84.16.110.044435Isopropyl ether6.72.30.77.044436Methyl acetate7.63.53.79.134437Methyl acetate7.63.53.79.134448N-methyl-2-pyrolidone8.86.03.511.211339Methylene hloride8.93.13.09.924441Nitrobenzene9.84.22.010.914442Nitrobenzene9.84.22.010.91	24	Dimethyl sulfoxide	9.0	8.0	5.0	13.0	1	1	2 1
LabL	25	1 4-Diovane	9.3	0.0	3.6	10.0	3	3	2
25District1.74.53.510.415.411227Ethanol amine8.47.610.415.4111228Ethyl acetate7.72.63.58.8444292-Ethyl hexanol7.81.65.89.944420Ethyl cellocolve7.94.57.011.5422331Formic acid7.05.88.112.212332n-Hexamethyl phosphoramide9.04.25.511.314433n-Hexamethyl phosphoramide9.04.25.511.314434Isoamyl alcohol6.84.16.110.044435Isoproyl ether6.72.30.77.044436Methyl acetate7.63.53.79.134437Methyl ethyl ketone7.84.42.59.324438N-methyl-2-pyrolidone8.86.03.511.211339Methylenchloride8.93.13.09.924440Nitrobenzene9.84.22.010.914441Nitrobenzene9.84.22.010.914442Nitrobenzen	20	Fthanol	77	4.3	9.5	13.0	3	0	0 1
21Differ3.41.01.0.4	20 97	Ethanol amine	8.4	7.6	9.5 10.4	15.0	J 1	2	1
20Dury actuate1.12.03.0 $6.5$ $4$ $4$ $4$ $4$ 30Ethyl cellocolve7.9 $4.5$ 7.0 $11.5$ $4$ $2$ $2$ 31Formic acid7.0 $5.8$ $8.1$ $12.2$ $1$ $2$ $3$ 32 $n$ -Heptane7.2 $0.0$ $0.72$ $4$ $4$ $4$ 33 $n$ -Hexamethyl phosphoramide $9.0$ $4.2$ $5.5$ $11.3$ $1$ $4$ $4$ 34Isoarpyl actoact $6.7$ $2.3$ $0.7$ $7.0$ $4$ $4$ $4$ 35Isoproyl ether $6.7$ $2.3$ $0.7$ $7.0$ $4$ $4$ $4$ 36Methyl actate $7.6$ $3.5$ $3.7$ $9.1$ $3$ $4$ $4$ 37Methyl hetone $7.8$ $4.4$ $2.5$ $9.3$ $2$ $4$ $4$ 38N-methyl-2-pyrolidone $8.8$ $6.0$ $3.5$ $11.2$ $1$ $1$ $3$ 39Methylene chloride $8.9$ $3.1$ $3.0$ $9.9$ $2$ $4$ $4$ $41$ Nitrobenzene $7.8$ $7.6$ $2.2$ $11.1$ $1$ $4$ $4$ $44$ $1$ -Propanol $7.8$ $3.6$ $5.2$ $12.0$ $1$ $4$ $4$ $44$ $1$ -Propanol $7.8$ $3.6$ $5.2$ $12.0$ $1$ $4$ $4$ $44$ $1$ -Propanol $7.8$ $3.8$ $8.6$ $0.13.3$ $1$ $4$ $4$ <td>21</td> <td>Ethallor annie</td> <td>77</td> <td>2.0</td> <td>25</td> <td>10.4</td> <td>1</td> <td>1</td> <td>2</td>	21	Ethallor annie	77	2.0	25	10.4	1	1	2
2.52.52.51.63.63.944430Ethyl cellocolve7.94.57.011.542231Formic acid7.05.88.112.212332 $n$ -Heptane7.20.00.07.244433 $n$ -Hexamethyl phosphoramide9.04.25.511.314434Isoamyl alcohol6.84.16.110.044435Isopropyl ether6.72.30.77.044436Methyl acetate7.63.53.79.134437Methyl ketone7.84.42.59.324438N-methyl-2-pyrolidone8.86.03.511.211339Methylene chloride8.93.13.09.924441Nitrobenzene9.84.22.010.914442Nitromethane7.79.22.512.014443 $n$ -Octyl alcohol6.93.45.39.3444441-Propanol7.83.38.512.0144441-Propanol7.83.38.512.043245Propylene carbonate9.88.82.013.3 </td <td>20</td> <td>2. Ethyl hexenol</td> <td>7.1</td> <td>1.6</td> <td>5.0</td> <td>0.0</td> <td>4</td> <td>4</td> <td>4</td>	20	2. Ethyl hexenol	7.1	1.6	5.0	0.0	4	4	4
50Entry feributive1.34.31.31.342231Formic acid7.05.88.11.2.212332 $n$ -Heptane7.20.00.07.244433 $n$ -Hexamethyl phosphoramide9.04.25.511.314434Isoamyl alcohol6.84.16.110.044435Isopropyl ether6.72.30.77.044436Methyl acetate7.63.53.79.134437Methyl ethyl ketone7.84.42.59.324438N-methyl-2-pyrolidone8.86.03.511.211339Methylene chloride8.93.13.09.924440Nitrobenzene9.84.22.010.914441Nitrobethane7.79.22.512.014442Nitrobethane7.87.62.211.1144441-Propanol7.83.38.512.043245Propylene carbonate9.88.82.013.3144441-Propanol7.83.38.512.043245Propylene glycol8.24.011.	20	Ethyl cellocolye	7.0	1.0	5.8 7.0	9.9 11 5	4	4	4
31 $n$ -Heptane $7.0$ $0.3$ $0.1$ $12.2$ $1$ $2$ $3$ $32$ $n$ -Heptane $7.2$ $0.0$ $0.0$ $7.2$ $4$ $4$ $4$ $33$ $n$ -Hexamethyl phosphoramide $9.0$ $4.2$ $5.5$ $11.3$ $1$ $4$ $4$ $34$ Isoarnyl alcohol $6.8$ $4.1$ $6.1$ $10.0$ $4$ $4$ $4$ $35$ Isoproyl ether $6.7$ $2.3$ $0.7$ $7.0$ $4$ $4$ $4$ $36$ Methyl acetate $7.6$ $3.5$ $3.7$ $9.1$ $3$ $4$ $4$ $37$ Methyl ethyl ketone $7.8$ $4.4$ $2.5$ $9.3$ $2$ $4$ $4$ $38$ $N$ -methyl-2-pyrolidone $8.8$ $6.0$ $3.5$ $11.2$ $1$ $1$ $3$ $39$ Methylene chloride $8.9$ $3.1$ $3.0$ $9.9$ $2$ $4$ $4$ $40$ Nitrobenzene $9.8$ $4.2$ $2.0$ $10.9$ $1$ $4$ $4$ $41$ Nitrobethane $7.7$ $9.2$ $2.5$ $12.0$ $1$ $4$ $4$ $42$ Nitromethane $7.8$ $3.3$ $8.5$ $2.0$ $4$ $3$ $2$ $45$ Propylene carbonate $9.8$ $8.2$ $2.0$ $13.3$ $1$ $4$ $4$ $46$ Propylene glycol $8.2$ $4.0$ $11.4$ $14.8$ $4$ $4$ $47$ Pyridine $9.3$ $4.3$ $2.9$ $10.7$ <t< td=""><td>31</td><td>Echyl cenocolve</td><td>7.0</td><td>4.0</td><td>9.1</td><td>11.0</td><td>4</td><td>2</td><td>2</td></t<>	31	Echyl cenocolve	7.0	4.0	9.1	11.0	4	2	2
32       n-Heyamethyl phosphoramide       9.0       4.2       5.5       11.3       1       4       4         33       n-Hexamethyl phosphoramide       9.0       4.2       5.5       11.3       1       4       4         34       Isoamyl alcohol       6.8       4.1       6.1       10.0       4       4       4         35       Isopropyl ether       6.7       2.3       0.7       7.0       4       4       4         36       Methyl acetate       7.6       3.5       3.7       9.1       3       4       4         37       Methyl ethyl ketone       7.8       4.4       2.5       9.3       2       4       4         38       N-methyl-2-pyrolidone       8.8       6.0       3.5       11.2       1       1       3         39       Methylene chloride       8.9       3.1       3.0       9.9       2       4       4         40       Nitrobenzene       9.8       4.2       2.0       10.9       1       4       4         41       Nitroethane       7.7       9.2       2.5       12.0       1       4       4         42       Nitromethane </td <td>20</td> <td>r Hontono</td> <td>7.0</td> <td>0.0</td> <td>0.1</td> <td>12.2</td> <td>1</td> <td>2</td> <td>3</td>	20	r Hontono	7.0	0.0	0.1	12.2	1	2	3
35 $h^{21}$ (example inversion index5.04.25.311.314434Isoamyl alcohol6.84.16.110.044435Isopropyl ether6.72.30.77.044436Methyl acetate7.63.53.79.134437Methylethyl ketone7.84.42.59.324438N-methyl-2-pyrolidone8.86.03.511.211339Methylene chloride8.93.13.09.924440Nitrobenzene9.84.22.010.914441Nitroethane7.79.22.512.014442Nitromethane7.79.22.512.014443 $n$ -Octyl alcohol6.93.43.38.512.0432441-Propanol7.83.38.512.043245Propylene carbonate9.88.82.013.314446Propylene glycol8.24.011.414.84447Pyridine9.34.32.910.711248Styrene9.10.5223350Tetrahydrofuran8.22.83.9	02 99	n Horomothyl phoophoromide	1.2	4.9	0.0	1.4	4	4	4
34Isoanyr atom $6.3$ $4.1$ $6.1$ $10.0$ $4$ $4$ $4$ $4$ $35$ Isopropyl ether $6.7$ $2.3$ $0.7$ $7.0$ $4$ $4$ $4$ $36$ Methyl acetate $7.6$ $3.5$ $3.7$ $9.1$ $3$ $4$ $4$ $37$ Methyl ethyl ketone $7.8$ $4.4$ $2.5$ $9.3$ $2$ $4$ $4$ $38$ N-methyl-2-pyrolidone $8.8$ $6.0$ $3.5$ $11.2$ $1$ $1$ $3$ $39$ Methylene chloride $8.9$ $3.1$ $3.0$ $9.9$ $2$ $4$ $4$ $40$ Nitrobenzene $9.8$ $4.2$ $2.0$ $10.9$ $1$ $4$ $4$ $41$ Nitroethane $7.7$ $9.2$ $2.5$ $12.0$ $1$ $4$ $4$ $42$ Nitromethane $7.7$ $9.2$ $2.5$ $12.0$ $1$ $4$ $4$ $43$ $n$ -Octyl alcohol $6.9$ $3.4$ $5.3$ $9.3$ $4$ $4$ $4$ $44$ $1$ -Propanol $7.8$ $3.3$ $8.5$ $12.0$ $4$ $3$ $2$ $45$ Propylene glycol $8.2$ $4.0$ $11.4$ $14.8$ $4$ $4$ $4$ $46$ Propylene glycol $8.2$ $4.0$ $11.4$ $14.8$ $4$ $4$ $47$ Pyridine $9.3$ $4.3$ $2.9$ $10.7$ $1$ $1$ $2$ $48$ Styrene $9.1$ $0.5$ $2.0$ $9.3$ $4$	24		9.0	4.2	0.0	11.3	1	4	4
55Isopopylether6.72.5 $0.7$ $7.0$ $4$ $4$ $4$ 36Methyl actate7.6 $3.5$ $3.7$ $9.1$ $3$ $4$ $4$ 37Methyl ethyl ketone7.8 $4.4$ $2.5$ $9.3$ $2$ $4$ $4$ 38N-methyl-2-pyrolidone $8.8$ $6.0$ $3.5$ $11.2$ $1$ $1$ $3$ 39Methylene chloride $8.9$ $3.1$ $3.0$ $9.9$ $2$ $4$ $4$ 40Nitrobenzene $9.8$ $4.2$ $2.0$ $10.9$ $1$ $4$ $4$ 41Nitroethane $7.8$ $7.6$ $2.2$ $11.1$ $1$ $4$ $4$ 42Nitromethane $7.7$ $9.2$ $2.5$ $12.0$ $1$ $4$ $4$ 43 $n$ -Octyl alcohol $6.9$ $3.4$ $5.3$ $9.3$ $4$ $4$ $4$ 44 $1$ -Propanol $7.8$ $3.3$ $8.5$ $12.0$ $4$ $3$ $2$ 45Propylene carbonate $9.8$ $8.8$ $2.0$ $13.3$ $1$ $4$ $4$ 46Propylene glycol $8.2$ $4.0$ $11.4$ $14.8$ $4$ $4$ 47Pyridine $9.3$ $4.3$ $2.9$ $10.7$ $1$ $1$ $2$ 48Styrene $9.1$ $0.5$ $2.0$ $9.3$ $4$ $4$ $4$ 49Tetrahydrofuran $8.2$ $2.8$ $3.9$ $9.5$ $2$ $2$ $2$ $3$	04 95	Isoamyi alconoi	0.0	4.1	0.1	10.0	4	4	4
30       Methyl acetate       7.6       3.7       9.1       3       4       4         37       Methyl acetate       7.8       4.4       2.5       9.3       2       4       4         38       N-methyl-2-pyrolidone       8.8       6.0       3.5       11.2       1       1       3         39       Methylene chloride       8.9       3.1       3.0       9.9       2       4       4         40       Nitrobenzene       9.8       4.2       2.0       10.9       1       4       4         41       Nitroethane       7.8       7.6       2.2       11.1       1       4       4         42       Nitromethane       7.7       9.2       2.5       12.0       1       4       4         43       n-Octyl alcohol       6.9       3.4       5.3       9.3       4       4       4         44       1-Propanol       7.8       3.3       8.5       12.0       4       3       2         45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         47       Pyridine       9.3       4.3       2.	30 90	Nothel costate	0.7	2.3	0.7	7.0	4	4	4
37       Methyl etnyl ketone       7.8       4.4       2.5       9.3       2       4       4         38       N-methyl-2-pyrolidone       8.8       6.0       3.5       11.2       1       1       3         39       Methylen chloride       8.9       3.1       3.0       9.9       2       4       4         40       Nitrobenzene       9.8       4.2       2.0       10.9       1       4       4         41       Nitroethane       7.8       7.6       2.2       11.1       1       4       4         42       Nitromethane       7.7       9.2       2.5       12.0       1       4       4         43 <i>n</i> -Octyl alcohol       6.9       3.4       5.3       9.3       4       4       4         44       1-Propanol       7.8       3.3       8.5       12.0       4       3       2         45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         46       Propylene glycol       8.2       4.0       11.4       14.8       4       4         47       Pyridine       9.3       4.3	00 07	Methyl athal betar	7.0	3.5	3.7	9.1	3	4	4
35       N-methyl-2-pyrolidone       8.8       6.0       3.5       11.2       1       1       3         39       Methylene chloride       8.9       3.1       3.0       9.9       2       4       4         40       Nitrobenzene       9.8       4.2       2.0       10.9       1       4       4         41       Nitrobenzene       9.8       7.6       2.2       11.1       1       4       4         42       Nitromethane       7.7       9.2       2.5       12.0       1       4       4         43       n-Octyl alcohol       6.9       3.4       5.3       9.3       4       4       4         44       1-Propanol       7.8       3.3       8.5       12.0       4       3       2         45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         46       Propylene glycol       8.2       4.0       11.4       14.8       4       4         47       Pyridine       9.3       4.3       2.9       10.7       1       1       2         48       Styrene       9.1       0.5       2	37 90	Meethyl ethyl Recone	1.0	4.4	2.5	9.3	2	4	4
359Methylehe chloride8.93.13.09.924440Nitrobenzene9.84.22.010.914441Nitroethane7.87.62.211.114442Nitromethane7.79.22.512.014443 <i>n</i> -Octyl alcohol6.93.45.39.3444441-Propanol7.83.38.512.043245Propylene carbonate9.88.82.013.314446Propylene glycol8.24.011.414.84447Pyridine9.34.32.910.711248Styrene9.10.52.09.344449Tetrahydrofuran8.22.83.99.522350Tetralin9.61.01.49.844451Tetramethylurea8.24.05.410.6114521,1,1-Trichloroethane8.32.11.08.744453Triethyl phosphate8.27.85.012.411354Toluene8.80.71.09.1444	30 20	Notherland shlarida	8.8	0.0	3.5	11.z	1	1	3
40Nitrobenzene9.84.22.010.914441Nitroethane7.87.62.211.114442Nitromethane7.79.22.512.014443n-Octyl alcohol6.93.45.39.3444441-Propanol7.83.38.512.043245Propylene carbonate9.88.82.013.314446Propylene glycol8.24.011.414.84447Pyridine9.34.32.910.711248Styrene9.10.52.09.344449Tetrahydrofuran8.22.83.99.522350Tetrain9.61.01.49.844451Tetramethylurea8.24.05.410.6114521,1,1-Trichloroethane8.32.11.08.744453Triethyl phosphate8.25.64.510.911354Trimethyl phosphate8.27.85.012.411355Toluene8.80.71.09.1444	39	Methylene chloride	8.9	3.1	3.0	9.9	2	4	4
41       Nitroethane       7.8       7.6       2.2       11.1       1       4       4         42       Nitromethane       7.7       9.2       2.5       12.0       1       4       4         43       n-Octyl alcohol       6.9       3.4       5.3       9.3       4       4       4         44       1-Propanol       7.8       3.3       8.5       12.0       4       3       2         45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         46       Propylene glycol       8.2       4.0       11.4       14.8       4       4         47       Pyridine       9.3       4.3       2.9       10.7       1       1       2         48       Styrene       9.1       0.5       2.0       9.3       4       4       4         49       Tetrahydrofuran       8.2       2.8       3.9       9.5       2       2       3         50       Tetrain       9.6       1.0       1.4       9.8       4       4       4         51       Tetramethylurea       8.2       4.0       5.4 <td< td=""><td>40</td><td>Nitrobenzene</td><td>9.8</td><td>4.2</td><td>2.0</td><td>10.9</td><td>1</td><td>4</td><td>4</td></td<>	40	Nitrobenzene	9.8	4.2	2.0	10.9	1	4	4
42Nitromethane7.79.22.512.014443n-Octyl alcohol6.93.45.39.3444441-Propanol7.83.38.512.043245Propylene carbonate9.88.82.013.314446Propylene glycol8.24.011.414.844447Pyridine9.34.32.910.711248Styrene9.10.52.09.344449Tetrahydrofuran8.22.83.99.522350Tetrain9.61.01.49.844451Tetramethylurea8.24.05.410.6114521,1,1-Trichloroethane8.32.11.08.744453Triethyl phosphate8.25.64.510.911354Trimethyl phosphate8.27.85.012.411355Toluene8.80.71.09.1444	41	Nitroethane	7.8	7.6	2.2	11.1	1	4	4
43       n-Uctyl alcohol       6.9       3.4       5.3       9.3       4       4       4         44       1-Propanol       7.8       3.3       8.5       12.0       4       3       2         45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         46       Propylene glycol       8.2       4.0       11.4       14.8       4       4         47       Pyridine       9.3       4.3       2.9       10.7       1       1       2         48       Styrene       9.1       0.5       2.0       9.3       4       4       4         49       Tetrahydrofuran       8.2       2.8       3.9       9.5       2       2       3         50       Tetrain       9.6       1.0       1.4       9.8       4       4       4         51       Tetramethylurea       8.2       4.0       5.4       10.6       1       1       4         52       1,1,1-Trichloroethane       8.3       2.1       1.0       8.7       4       4       4         53       Triethyl phosphate       8.2       5.6       4.5	42	Nitromethane	7.7	9.2	2.5	12.0	1	4	4
44       1-Propanol       7.8       3.3       8.5       12.0       4       3       2         45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         46       Propylene glycol       8.2       4.0       11.4       14.8       4       4       4         47       Pyridine       9.3       4.3       2.9       10.7       1       1       2         48       Styrene       9.1       0.5       2.0       9.3       4       4       4         49       Tetrahydrofuran       8.2       2.8       3.9       9.5       2       2       3         50       Tetrain       9.6       1.0       1.4       9.8       4       4       4         51       Tetramethylurea       8.2       4.0       5.4       10.6       1       1       4         52       1,1,1-Trichloroethane       8.3       2.1       1.0       8.7       4       4       4         53       Triethyl phosphate       8.2       5.6       4.5       10.9       1       1       3         54       Trimethyl phosphate       8.2	43	n-Octyl alcohol	6.9	3.4	5.3	9.3	4	4	4
45       Propylene carbonate       9.8       8.8       2.0       13.3       1       4       4         46       Propylene glycol       8.2       4.0       11.4       14.8       4       4       4         47       Pyridine       9.3       4.3       2.9       10.7       1       1       2         48       Styrene       9.1       0.5       2.0       9.3       4       4       4         49       Tetrahydrofuran       8.2       2.8       3.9       9.5       2       2       3         50       Tetrain       9.6       1.0       1.4       9.8       4       4       4         51       Tetramethylurea       8.2       4.0       5.4       10.6       1       1       4         52       1,1,1-Trichloroethane       8.3       2.1       1.0       8.7       4       4       4         53       Triethyl phosphate       8.2       5.6       4.5       10.9       1       1       3         54       Trimethyl phosphate       8.2       7.8       5.0       12.4       1       1       3         55       Toluene       8.8       0.7	44	1-Propanol	7.8	3.3	8.5	12.0	4	3	2
46Propylene glycol8.24.011.414.844447Pyridine9.34.32.910.711248Styrene9.10.52.09.344449Tetrahydrofuran8.22.83.99.522350Tetrain9.61.01.49.844451Tetramethylurea8.24.05.410.6114521,1,1-Trichloroethane8.32.11.08.744453Triethyl phosphate8.25.64.510.911354Trimethyl phosphate8.27.85.012.411355Toluene8.80.71.09.1444	45	Propylene carbonate	9.8	8.8	2.0	13.3	1	4	4
47Pyridine $9.3$ $4.3$ $2.9$ $10.7$ $1$ $1$ $2$ $48$ Styrene $9.1$ $0.5$ $2.0$ $9.3$ $4$ $4$ $4$ $49$ Tetrahydrofuran $8.2$ $2.8$ $3.9$ $9.5$ $2$ $2$ $3$ $50$ Tetralin $9.6$ $1.0$ $1.4$ $9.8$ $4$ $4$ $4$ $51$ Tetramethylurea $8.2$ $4.0$ $5.4$ $10.6$ $1$ $1$ $4$ $52$ $1,1,1$ -Trichloroethane $8.3$ $2.1$ $1.0$ $8.7$ $4$ $4$ $4$ $53$ Triethyl phosphate $8.2$ $5.6$ $4.5$ $10.9$ $1$ $1$ $3$ $54$ Trimethyl phosphate $8.2$ $7.8$ $5.0$ $12.4$ $1$ $1$ $3$ $55$ Toluene $8.8$ $0.7$ $1.0$ $9.1$ $4$ $4$ $4$	46	Propylene glycol	8.2	4.0	11.4	14.8	4	4	4
48       Styrene       9.1       0.5       2.0       9.3       4       4       4         49       Tetrahydrofuran       8.2       2.8       3.9       9.5       2       2       3         50       Tetralin       9.6       1.0       1.4       9.8       4       4       4         51       Tetramethylurea       8.2       4.0       5.4       10.6       1       1       4         52       1,1,1-Trichloroethane       8.3       2.1       1.0       8.7       4       4       4         53       Triethyl phosphate       8.2       5.6       4.5       10.9       1       1       3         54       Trimethyl phosphate       8.2       7.8       5.0       12.4       1       1       3         55       Toluene       8.8       0.7       1.0       9.1       4       4       4	47	Pyridine	9.3	4.3	2.9	10.7	1	1	2
49       Tetrahydrofuran       8.2       2.8       3.9       9.5       2       2       3         50       Tetralin       9.6       1.0       1.4       9.8       4       4       4         51       Tetramethylurea       8.2       4.0       5.4       10.6       1       1       4         52       1,1,1-Trichloroethane       8.3       2.1       1.0       8.7       4       4       4         53       Triethyl phosphate       8.2       5.6       4.5       10.9       1       1       3         54       Trimethyl phosphate       8.2       7.8       5.0       12.4       1       1       3         55       Toluene       8.8       0.7       1.0       9.1       4       4       4	48	Styrene	9.1	0.5	2.0	9.3	4	4	4
50Tetralin9.61.01.49.844451Tetramethylurea8.24.05.410.6114521,1,1-Trichloroethane8.32.11.08.744453Triethyl phosphate8.25.64.510.911354Trimethyl phosphate8.27.85.012.411355Toluene8.80.71.09.1444	49	Tetrahydrofuran	8.2	2.8	3.9	9.5	2	2	3
51Tetramethylurea8.24.05.410.6114521,1,1-Trichloroethane8.32.11.08.744453Triethyl phosphate8.25.64.510.911354Trimethyl phosphate8.27.85.012.411355Toluene8.80.71.09.1444	50	Tetralin	9.6	1.0	1.4	9.8	4	4	4
52       1,1,1-Trichloroethane       8.3       2.1       1.0       8.7       4       4       4         53       Triethyl phosphate       8.2       5.6       4.5       10.9       1       1       3         54       Trimethyl phosphate       8.2       7.8       5.0       12.4       1       1       3         55       Toluene       8.8       0.7       1.0       9.1       4       4       4	51	Tetramethylurea	8.2	4.0	5.4	10.6	1	1	4
53       Triethyl phosphate       8.2       5.6       4.5       10.9       1       1       3         54       Trimethyl phosphate       8.2       7.8       5.0       12.4       1       1       3         55       Toluene       8.8       0.7       1.0       9.1       4       4       4	52	1,1,1-Trichloroethane	8.3	2.1	1.0	8.7	4	4	4
54         Trimethyl phosphate         8.2         7.8         5.0         12.4         1         1         3           55         Toluene         8.8         0.7         1.0         9.1         4         4         4	53	Triethyl phosphate	8.2	5.6	4.5	10.9	1	1	3
55         Toluene         8.8         0.7         1.0         9.1         4         4         4	54	Trimethyl phosphate	8.2	7.8	5.0	12.4	1	1	3
	55	Toluene	8.8	0.7	1.0	9.1	4	4	4

Table IExtent of Solubility of PMAN, PMAA, and MAN/MAA Copolymer in Liquids: Good Solvent (1),Good Swelling Agent (2), Poor Swelling Agent (3), and Nonsolvent (4)

# **RESULTS AND DISCUSSION**

#### **Homopolymer PMAN**

The solubility region of homopolymer PMAN in the Hansen 3-dimensional space as wel as the total solubility parameter composed of dispersion  $(\delta_{d,p})$ , polar  $(\delta_{p,p})$ , and hydrogen bonding  $(\delta_{h,p})$  components has been determined as follows. Each liquid used for solubility experiments is represented as a point on a three-dimensional plot with  $\delta_d$ ,  $\delta_p$ , and  $\delta_h$  as axes. The scale of  $\delta_d$  is twice as that used for  $\delta_p$  and  $\delta_h$ .

The boundaries of the solubility region for each of the  $\delta_d - \delta_p$ ,  $\delta_d - \delta_h$ , and  $\delta_p - \delta_h$  planes have been drawn in such a way to include all the good solvents and exclude all the nonsolvents as well as poor swelling agents, with good swelling agents at the boundaries. The analytical representation of the solubility region in the Hansen three-dimensional space is obtained by a computer iteration based on the linear regression method. The solubility region in the Hansen space is represented by the equation

$$4(\delta_d - \delta_{d,p})^2 + (\delta_p - \delta_{p,p})^2 + (\delta_h - \delta_{h,p})^2 = 5.0^2$$
(3)

where the parameters with subscript p referred to the coordinates of the center of the spheroid, which correspond to the solubility parameter components of PMAN and the solubility sphere of radius in Hansen space is 5.0. Thus, the following values have been obtained for PMAN:  $\delta_{d,p} = 8.8$ ,  $\delta_{p,p} = 7.8$ , and  $\delta_{h,p} = 3.9 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ . According to eq. (4)

$$\delta_{t,p}^{2} = \delta_{d,p}^{2} + \delta_{p,p}^{2} + \delta_{h,p}^{2}$$
(4)

the total solubility parameter  $\delta_{t,p}$  is 12.4 cal<sup>1/2</sup> cm<sup>-3/2</sup>.

Alternatively theoretical and semiempirical methods could be used to evaluate the polymer solubility parameter as well. Among them, the group contribution method is widely used. Based on an examination of a vast amount of data on simple liquids, Fedors<sup>12</sup> found that a general system for estimating both energy of vaporization,  $E_v$ , and molar volume, V, could be set up simply by assuming equations as

$$E_{v} = \sum_{i} \Delta e_{i} \tag{5}$$

$$V = \sum_{i} \Delta V_{i} \tag{6}$$

where  $\Delta e_i$  and  $\Delta V_i$  are the additive atomic and group contribution for the energy of vaporization and molar volume, respectively.

Using eqs. (5) and (6), the total solubility parameter of high molecular polymer becomes

$$\delta_t = \left(\frac{\sum_i E_i}{\sum_i V_i}\right)^{1/2} \tag{7}$$

where  $E_i$  and  $V_i$  are the additive atomic and group contribution of the repeating unit for the energy of vaporization and molar volume, respectively. The group contribution of  $E_i$  and  $V_i$  taken from the Fedors<sup>12</sup> for PMAN are shown in Table II. Then, the total solubility parameter is evaluated according to eq. (7)

$$\delta_t = \left(\frac{\sum_i E_i}{\sum_i V_i}\right)^{1/2} = \left(\frac{8755}{54.4}\right)^{1/2} = 12.6 \text{ cal}^{1/2} \text{ cm}^{-3/2}$$

Using the molar attraction constant in conjunction with eq. (7), the total solubility parameter can be written as

$$\delta_t = \frac{\sum_i F_i}{\sum_i V_i} \tag{8}$$

where  $F_i$  are the additive atomic and group contribution of the repeating unit for the molar attraction constant. Hoy<sup>14</sup> and Van Krevelen<sup>15</sup> also derived a set of atomic contribution  $F_i$  to calculate  $\delta_t$ . By using the  $F_i$  values collected in Table III and using eq.

Table II Group Contribution to Energy of Vaporization  $E_i$  and Molar Volume  $V_i$ Taken from Fedors<sup>12</sup>

-	$E_i$	$V_i$
Group	(cal/mol)	(cm°/mol)
–CH₃	1125	33.5
$-CH_2-$	1180	16.1
 C 	351	-19.2
-CN	6099	24.0
-COOH	6600	28.5

Tabl	eIII (	Group	Contribution	n to F <sub>i</sub>	(cal'/* c	2m <sup>3/2</sup> /
mol)	Taken	from	Literature <sup>13</sup>	-15		

	$F_i$				
Group	Small	Van Krevelen	Hoy		
-CH3	104	100	72.5		
CH <sub>2</sub>	64.8	66.9	64.3		
 C	-45.4	0.0	15.6		
-CN	200	234.6	173.3		
—СООН		155.8	238.9		

(8), we find 10.4 cal<sup>1/2</sup> cm<sup>-3/2</sup> <  $\delta_{t,p}$  < 12.8 cal<sup>1/2</sup> cm<sup>-3/2</sup> for PMAN.

The group contribution method is also applicable to evaluate dispersion, polar and hydrogen bonding components.<sup>19,20</sup> By direct analogy to eqs. (7) and (8), it follows that:

$$\delta_{d,p} = \frac{\sum_{i} F_{di}}{\sum_{i} V_{i}}$$
(9a)

$$\delta_{p,p} = \frac{\left(\sum_{i} F_{pi}^{2}\right)^{1/2}}{\sum_{i} V_{i}}$$
(9b)

$$\delta_{h,p} = \left(\frac{\sum_{i} E_{hi}}{\sum_{i} V_{i}}\right)^{1/2}$$
(9c)

where  $F_{di}$ ,  $F_{pi}$ , and  $E_{hi}$  are the molar attraction constants for dispersion, polar, and hydrogen bonding

Table V Comparison of Experimental and Calculated Solubility Parameters  $(cal^{1/2} cm^{-3/2})$  of PMAN

Method	$\delta_{d,p}$	$\delta_{p,p}$	$\delta_{h,p}$	$\delta_{t,p}$
Experiment	8.8	7.8	3.9	12.4
Group contribution	_			12.6*
<i>P</i>			—	10.4 <sup>b</sup>
			_	12.8°
	_		_	$10.4^{d}$
	8.0	8.4	3.0	12.0°

<sup>a</sup> Calculated from Fedors method.

<sup>b</sup> Calculated from Small method.

<sup>c</sup> Calculated from Van Krevelen method.

<sup>d</sup> Calculated from Hoy method.

<sup>e</sup> Calculated from solubility parameter component group contribution method.

forces, respectively. The group contribution of the molar attraction constants of  $F_{di}$ ,  $F_{pi}$ , and  $E_{hi}$  taken from the literature <sup>19,20</sup> are shown in Table IV. According to eqs. (4) and (9), the values of the solubility parameter and its components are:  $\delta_{d,p} = 8.0$ ,  $\delta_{p,p} = 8.4$ ,  $\delta_{h,p} = 3.1$ , and  $\delta_{t,p} = 12.0 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ .

All the experimental and calculated solubility parameters for PMAN are collected in Table V. It appears that they are in good agreement.

## **Homopolymer PMAA**

Homopolymer PMAA does not dissolve in any liquid but only swells in some of them at 25°C. After raising the temperature to 70°C, three good solvents were found for PMAA, namely: diethylene glycol, dimethyl sulfoxide, and ethanol.

 Table IV
 Solubility Parameter Component Group Contribution from Literature<sup>19,20</sup>

Group	$\frac{F_{di}}{(\mathrm{cal}^{1/2}~\mathrm{cm}^{3/2}/\mathrm{mol})}$	$F_{pi} \ ({ m cal}^{1/2} \ { m cm}^{3/2}/{ m mol})$	$E_{hi}$ (cal/mol)
-CH <sub>3</sub>	205	0.0	0.0
$-CH_2-$	132	0.0	0.0
	-34.2	0.0	0.0
-CN	210	537.6	597
—СООН	259	205	2389

Following the same procedures described in the previous section, the solubility envelope of the PMAA in the Hansen space as well as the values of the solubility parameters have been determined. The solubility of PMAA in terms of Hansen parameters is represented by a spheroid, best fitted by equation

$$4(\delta_d - \delta_{d,p})^2 + (\delta_p - \delta_{p,p})^2 + (\delta_h - \delta_{h,p})^2 = 3.0^2.$$
(10)

The individual parameters of PMAA thus obtained are:  $\delta_{d,p} = 8.5$ ,  $\delta_{p,p} = 6.1$ ,  $\delta_{h,p} = 7.8$ , and  $\delta_{t,p} = 13.1$  cal<sup>1/2</sup> cm<sup>-3/2</sup>.

The solubility parameters of PMAA have been calculated on the basis of the group contribution method. By using the  $E_i$ ,  $F_i$ ,  $F_{di}$ ,  $F_{pi}$ , and  $E_{hi}$  values collected in Tables II to IV, and using the eqs. (4) and (7) to (9), we obtain 9.1 cal<sup>1/2</sup> cm<sup>-3/2</sup> <  $\delta_{t,p}$  < 12.5 cal<sup>1/2</sup> cm<sup>-3/2</sup>,  $\delta_{d,p} = 8.5$ ,  $\delta_{p,p} = 3.1$ , and  $\delta_{h,p} = 6.0$  cal<sup>1/2</sup> cm<sup>-3/2</sup>. Table VI lists the experimental and calculated values for PMAA. It appeared that our experimental results were higher than the calculated values, except the value of the dispersion solubility parameter  $\delta_{d,p}$ .



**Figure 1** The solubility regions of PMAN, PMAA, and their copolymer in the  $\delta_d - \delta_p$  plane.

# MAN/MAA Copolymer

The solubility region of MAN/MAA copolymer in the Hansen space is represented by equation

$$4(\delta_d - \delta_{d,p})^2 + (\delta_p - \delta_{p,p})^2 + (\delta_h - \delta_{h,p})^2 = 3.9^2$$
(11)

The individual parameters of MAN/MAA copoly-

Table VIComparison of Experimental andCalculated Solubility Parameters(cal<sup>1/2</sup> cm<sup>-3/2</sup>) of PMAA

Method	$\delta_{d,p}$	$\delta_{p,p}$	$\delta_{h,p}$	$\delta_{t,p}$
Experiment	8.5	6.1	7.8	13.1
Group contribution	_			12.5ª
*				10.4 <sup>b</sup>
	-	-		12.2°
	8.5	3.1	6.0	9.1 <sup>d</sup>

<sup>a</sup> Calculated from Fedors method.

<sup>b</sup> Calculated from Van Krevelen method.

<sup>d</sup> Calculated from Hoy method.

<sup>e</sup> Calculated from solubility parameter component group contribution method.



**Figure 2** The solubility regions of PMAN, PMAA, and their copolymer in the  $\delta_d - \delta_h$  plane.



**Figure 3** The solubility regions of PMAN, PMAA, and their copolymer in the  $\delta_p - \delta_h$  plane.

mer are:  $\delta_{d,p} = 8.5$ ,  $\delta_{p,p} = 7.0$ , and  $\delta_{h,p} = 6.0 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ . According to eq. (4), the total solubility parameter  $\delta_{t,p}$  is 12.6 cal<sup>1/2</sup> cm<sup>-3/2</sup>. From our experimental results, the solubility parameter of random copolymer MAN/MAA is between those of the homopolymer constituents as shown in Figures 1–3.

The solubility parameters for random copolymer can be predicted from data available for the homopolymers. It would appear that this could be done with the assumption that total solubility parameter of the copolymer is related with the components in terms of their volume fractions. It has the following relation <sup>19,20</sup>:

$${}^{ij}\delta_{t,p} = {}^{i}\phi^{i}\delta_{t,p} + {}^{j}\phi^{j}\delta_{t,p}$$
(12)

where  $\phi$  is the homopolymer volume fractions, superscript *i* and *j* referring to the components and *ij* referring to the copolymer. Equation (12) can be also applicable to evaluate  $\delta_{d,p}$ ,  $\delta_{p,p}$ , and  $\delta_{h,p}$ . By direct analogy with eq. (12) it follows that <sup>19,20</sup>:

Bernard Schneler<sup>21</sup> used an alternate method to calculate the  $\delta_{t,p}$  of random copolymer. He proposed that:

$${}^{ij}\delta_{t,p} = \frac{({}^{i}n {}^{i}M^{2}/{}^{i}\rho) {}^{i}\delta_{t,p} + ({}^{j}n {}^{j}M^{2}/{}^{j}\rho) {}^{i}\delta_{t,p}}{\{({}^{i}n {}^{i}M + {}^{j}n {}^{j}M)\}\{[({}^{i}n {}^{i}M^{2}/{}^{i}\rho) + ({}^{j}n {}^{j}M^{2}/{}^{j}\rho)][1/{}^{ij}\rho]\}^{1/2}}$$
(14)

where n, M, and  $\rho$  refer to number of moles, monomer molecular weight, and density, respectively. The same relationship can also be used to evaluate  $\delta_{d,p}$ ,  $\delta_{p,p}$ , and  $\delta_{h,p}$  as follows:

Experimental results and calculated values are summarized in Table VII. It appears that they are in good agreement. However, calculated solubility parameters of MAN/MAA copolymer based on the calculated values of the homopolymers are lower than the experimental results.

# CONCLUSIONS

Solubility tests have been carried out to evaluate the solubility parameters of PMAN and PMAA homopolymers and MAN/MAA copolymer. The solubility behavior of PMAN, PMAA, and MAN/MAA copolymer have been examined in about 55 liquids. The theoretical values of the solubility parameters calculated from the group contribution method are in good agreement with the experimental results for PMAN, but appear to be low for PMAA and MAN/ MAA copolymer. The solubility parameters of MAN/MAA copolymer obtained either by experiment or by calculation were intermediate between those of the homopolymer constituents PMAN and PMAA. Methods to predict solubility parameters of

Method	$\delta_{d,p}$	$\delta_{p,p}$	$\delta_{h,p}$	$\delta_{t,p}$
Experiment	8.5	7.0	6.0	12.6
(I) <sup>a</sup>	8.66	6.98	5.78	12.74°
. ,		_		$12.55^{d}$
				11.64°
	·			$11.27^{\rm f}$
	8.24	5.85	4.45	10.6 <sup>g</sup>
(II) <sup>b</sup>	8.64	6.87	6.03	12.78°
· · /				$12.54^{d}$
		_		11.48°
		_		$11.38^{f}$
	8.27	5.5	4.64	10.42 <sup>g</sup>

Table VII Comparison of Experimental and Calculated Solubility Parameters  $(cal^{1/2} cm^{-3/2})$ of MAN/MAA Copolymer

<sup>a</sup> Calculated from eqs. (12) and (13).

<sup>b</sup> Calculated from eqs. (14) and (15).

<sup>c</sup> Data of PMAN and PMAA calculated from our experimental results.

<sup>d</sup> Data of PMAN and PMAA calculated from Fedors method.

<sup>e</sup> Data of PMAN and PMAA calculated from Van Krevelen method.

<sup>f</sup> Data of PMAN and PMAA calculated from Hoy method.

<sup>g</sup> Data of PMAN and PMAA calculated from solubility parameter component group contribution method.

copolymer via known value of homopolymer constituents were justified by comparing with experimental results.

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