

Table of common included solvents. (1997)

Solvents sorted in order of percentage of the included solvent found in the Cambridge Data Base (1997) [Allen, F.H., Kennard, O. Chemical Design Automation News (1993) **8**, 31-37; Wilson A.J.C. (1988) **A44**, 715-724]. The percentage of disorder indicates how many structures of those that contain the included solvent are disordered.

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| Solvent            | Formula   | Total% | Disorder% |
|--------------------|---|--------|-----------|
| water              | HOH   | 8.8    | 24.7      |
| methylene chloride | H <sub>2</sub> CCl <sub>2</sub>                                 | 2.2    | 44.3      |
| methonal           | CH <sub>3</sub> OH  | 1.0    | 36.3      |
| benzene            | C <sub>6</sub> H <sub>6</sub>                                   | 1.0    | 24.4      |
| acetonitrile       | CH <sub>3</sub> CN  | 1.0    | 37.1      |
| toluene            | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                   | 0.87   | 61.6      |
| tetrahydrofuran    | (CH <sub>2</sub> ) <sub>4</sub> O                               | 0.81   | 48.7      |
| chloroform         | HCCL <sub>3</sub>   | 0.70   | 40.9      |
| ethanol            | CH <sub>3</sub> CH <sub>2</sub> OH                              | 0.62   | 54.0      |
| dimethylformide    | (CH <sub>3</sub> ) <sub>2</sub> CHO                             | 0.42   | 35.9      |
| ether              | (CH <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> O               | 0.40   | 57.2      |
| phenol             | C <sub>6</sub> H <sub>5</sub> OH                                | 0.3    | 21.1      |
| hexane             | CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub> | 0.23   | 59.8      |
| pyridine           | C <sub>5</sub> H <sub>5</sub> N                                 | 0.19   | 34.1      |
| dimethylsulfoxide  | (CH <sub>3</sub> ) <sub>2</sub> SO                              | 0.15   | 42.6      |

|                      |  |      |      |
|----------------------|--|------|------|
| dioxane              | $\text{O}(\text{CH}_2\text{CH}_2)_2\text{O}$   | 0.14 | 26.5 |
| ethyl acetate        | $\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_3$ | 0.11 | 48.4 |
| dichloroethane       | $\text{Cl}(\text{CH}_2)_2\text{Cl}$            | 0.08 | 45.5 |
| carbon tetrachloride | $\text{CCl}_4$                                 | 0.07 | 47.9 |
| cyclohexane          | $\text{C}_6\text{H}_{12}$                      | 0.06 | 58.8 |
| chlorobenzene        | $\text{C}_6\text{H}_5\text{Cl}$                | 0.06 | 47.5 |
| carbon disulfide     | $\text{CS}_2$                                  | 0.03 | 30.9 |
| iso-propanol         | $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$   | 0.02 | 47.5 |
| ethylene glycol      | $\text{HO}(\text{CH}_2)_2\text{OH}$            | 0.02 | 59.3 |