Microwave Absorption and Molecular Structure in Liquids. LXXIII. A Dielectric Study of Solute-Solvent Interactions¹

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Abstract: Measurements of dielectric constant and loss at 0.2, 1.2, 3.2, 10.0, and 25.0 cm have been made for seven chloroethanes in dilute cyclohexane, benzene, p-xylene, mesitylene, and p-dioxane solutions at 20-55°. The data have been used to calculate mean relaxation times and apparent dipole moments. For each ethane the mean relaxation time increases with increased solvent basicity, and an approximately linear relationship exists between the solute relaxation time and the ionization potential for the hydrocarbon solvents. In general, this behavior is interpreted in terms of weak solute-solvent interaction, probably C-H hydrogen bonding, hindering the rotation of the chloroethanes. The relative interactions for the solutes in each of the solvents capable of acting as proton acceptors are obtained by reference to their relaxation times in cyclohexane and may be expressed in terms of the increased free energies of activation for molecular rotation amounting to 150-850 cal/mol. In certain cases interaction is also evidenced by the solvent dependency of the apparent dipole moments.

xtensive work has been carried out on the subject of C-H groups as proton donors in hydrogen bonding.³ The potential of dielectric relaxation measurements as a method of studying weak molecular interactions has been illustrated for chloroform⁴ and for some haloethanes,^{5,6} whose relaxation times are appreciably longer in aromatic solvents than in cyclohexane or hexane, with which there is no specific interaction.⁷ So far the work has been limited to several haloethanes in cyclohexane and pxylene solutions at 25°6 and to 1,2-dichloroethane in cyclohexane, hexane, carbon tetrachloride, benzene, and *p*-xylene at $20^{\circ.5}$ Infrared spectroscopy, the most characteristic method for the detection of hydrogen bonding, is relatively insensitive to C-H--B hydrogen bonding, where B is a π -base proton acceptor. Thus, an extensive study of the dielectric behavior of the chloroethanes at low concentration to minimize solute-solute interactions, in nonpolar solvents capable of acting as proton acceptors (benzene, p-xylene, mesitylene, and p-dioxane) and an inert reference solvent (cyclohexane), was proposed. An additional object of this work was to investigate the effect of solvent upon the apparent dipole moment, which, in the case of 1,2-dichloroethane, is rather large.⁵

Experimental Section

Materials. The chloroethanes were all dried over calcium chloride prior to fractional distillation. Pentachloroethane and 1,1,2,2-tetrachloroethane were distilled under reduced pressure, and the small center fractions collected for use were stored in dark bottles over calcium chloride. Cyclohexane, benzene, p-xylene, and mesitylene were dried over and distilled from sodium. Dioxane was twice refluxed for 10 hr over sodium and then distilled from sodium.

Methods of Measurement. Dielectric constants and losses were measured at 0.20, 1.2, 3.2, 10.0, and 25.0 cm by methods which

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have been described previously.8-12 The static dielectric constants were measured at 575 m with a heterodyne beat apparatus.

The dielectric constants and losses for the solutions were corrected for the solvent absorptions which have been discussed elsewhere.13,14

Results

The measured values of the dielectric constants ε' and losses ε'' , which were considered too numerous for publication,¹⁵ were fed into an IBM 7094 computer programmed to solve the Cole-Cole equations¹⁶ for the most probable relaxation time τ_0 , distribution parameter α , and optical or infinite-frequency dielectric constant ε_{∞} .

Dipole moments were obtained from the Debye equation (eq 1) for dilute solutions in which ε_1 is the static

$$\mu = 0.01281 \left[\frac{3T(\varepsilon_0 - \varepsilon_{\infty})M_2}{(\varepsilon_1 + 2)^2 w_2 d_1} \right]^{1/2} \quad (1)$$

dielectric constant of the solvent, d_1 is its density, w_2 is the weight fraction of the solute, and M_2 is its molecular weight.

The free energy of activation difference $(\Delta \Delta G_0^*)$ for molecular reorientation in two solvents may be calculated using⁵ eq 2, in which τ_{0B} and τ_{0cyc} are the most probable

$$\tau_{0B}/\tau_{0eve} = \exp(\Delta \Delta G_0^{+}/RT)$$
 (2)

relaxation times in the solvents capable of acting as proton acceptors (benzene, *p*-xylene, mesitylene, and *p*-dioxane) and in cyclohexane, respectively.

Table I lists the most probable relaxation times (in picoseconds), distribution parameters, and dipole moments for the chloroethanes at mole fraction f_2 and temperature t in the different solvents. The calculated $\Delta\Delta G_0^{*}$ values are given in Table II.

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Table I. Most Probable Relaxation Times (τ_0) , Distribution Parameters (α) , and Dipole Moments (μ) for Chloroethanes at Mole Fraction (f_2) and Temperature (t) in Various Solvents

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Solvent	fa	t °C	τ_0	~	uЪ
$\begin{array}{c} 1,1=Dictor Orderhame \\ p-Xylene \\ 0,0254 \\ 25 \\ 2.7 \\ 0,028 \\ 25 \\ 4.7 \\ 0,028 \\ 25 \\ 5.8 \\ 0,021 \\ 0,0228 \\ 25 \\ 5.8 \\ 0,021 \\ 0,021 \\ 25 \\ 5.8 \\ 0,021 \\ 0,022 \\ 25 \\ 5.8 \\ 0,021 \\ 0,022 \\ 25 \\ 5.8 \\ 0,021 \\ 0,023 \\ 25 \\ 5.8 \\ 0,021 \\ 0,0423 \\ 55 \\ 1.6 \\ 0,066 \\ 1.44 \\ 0,0389 \\ 20 \\ 3.5 \\ 0,15 \\ 0,056 \\ 2.9 \\ 0,038 \\ 0,0389 \\ 50 \\ 2.9 \\ 0,03 \\ 0,0389 \\ 50 \\ 2.9 \\ 0,03 \\ 0,0389 \\ 50 \\ 2.9 \\ 0,03 \\ 0,0389 \\ 50 \\ 2.9 \\ 0,03 \\ 0,0389 \\ 0,0389 \\ 50 \\ 2.9 \\ 0,03 \\ 0,0389 \\ 0,0389 \\ 0,056 \\ 2.5 \\ 4.5 \\ 0,07 \\ 1.88 \\ 0,056 \\ 0.29 \\ 4.8 \\ 0,056 \\ 0.25 \\ 4.5 \\ 0,09 \\ 1.58 \\ 0,056 \\ 0.25 \\ 4.5 \\ 0,09 \\ 1.58 \\ 0,066 \\ 1.58 \\ 0,09 \\ 1.58 \\ 0,066 \\ 1.58 \\ 0,09 \\ 1.58 \\ 0,0643 \\ 2.5 \\ 3.3 \\ 0,09 \\ 1.58 \\ 0,008 \\ 1.51 \\ 0,0643 \\ 2.5 \\ 3.3 \\ 0,09 \\ 1.58 \\ 0,008 \\ 1.51 \\ 0,0643 \\ 2.5 \\ 5.3 \\ 0,008 \\ 1.51 \\ 0,0043 \\ 2.5 \\ 5.3 \\ 0,008 \\ 1.81 \\ 0,0024 \\ 55 \\ 2.7 \\ 0,06 \\ 1.87 \\ 0,0294 \\ 2.5 \\ 2.9 \\ 0,001 \\ 1.12 \\ -Trichloroethane \\ Cyclohexane \\ 0,0294 \\ 2.5 \\ 2.8 \\ 0,007 \\ 1.77 \\ 0,0495 \\ 5.5 \\ 3.2 \\ 0,06 \\ 1.87 \\ 0,0275 \\ 5.5 \\ 8 \\ 0,007 \\ 1.77 \\ 0,0495 \\ 5.5 \\ 1.2 \\ 0,007 \\ 1.77 \\ 0,0495 \\ 5.5 \\ 1.2 \\ 0,007 \\ 1.77 \\ 0,0495 \\ 5.5 \\ 1.2 \\ 0,008 \\ 1.81 \\ 0,075 \\ 5.8 \\ 0,007 \\ 1.77 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.81 \\ 0,007 \\ 1.77 \\ 0,0495 \\ 5.5 \\ 1.7 \\ 0,008 \\ 1.81 \\ 0,007 \\ 1.57 \\ 0,008 \\ 1.87 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,008 \\ 1.57 \\ 0,000 \\ 1.44 \\ 0,000 \\ 1.51 \\ 0,000 \\ 1.5$			Distilans	()300)		μ, D.
$\begin{array}{c} Cyclonexame 0, 0254 2.5 4.2 0, 002 1.88 \\ p-Xylene 0, 0265 2.5 4.5 0, 002 1.89 \\ Mesitylene 0, 0228 2.5 5.8 0, 002 1.98 \\ 1.2-Dichloroethame \\ Cyclohexame 0, 0228 2.5 5.8 0, 002 1.98 \\ 1.2-Dichloroethame \\ 0, 0463 2.0 2, 1 0, 10 1, 46 \\ Benzene 0, 0389 50 2, 9 0, 03 1, 76 \\ p-Xylene 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0560 2.5 4, 5 0, 07 1, 58 \\ 0, 0643 2.5 5, 3 0, 08 1, 51 \\ 0, 0643 2.5 5, 3 0, 08 1, 51 \\ 0, 0643 2.5 5, 3 0, 08 1, 82 \\ 0, 0232 2.5 5, 9 0, 07 1, 58 \\ 1, 1, 1-Trichloroethame \\ Cyclohexane 0, 0234 2.5 2, 9 0, 02 1, 84 \\ 0, 0294 5.5 2, 1 0, 06 1, 87 \\ Benzene 0, 0275 2.5 3, 7 0, 03 1, 82 \\ p-Xylene 0, 0417 2.5 4, 0 0, 07 1, 76 \\ 0, 0495 2.5 4, 8 0, 07 1, 77 \\ 0, 0495 2.5 4, 8 0, 07 1, 77 \\ p-Dioxane 0, 021 2.5 5, 8 0, 08 1, 81 \\ p-Dioxane 0, 0221 2.5 7, 1 0, 03 1, 87 \\ p-Dioxane 0, 0221 2.5 7, 1 0, 03 1, 57 \\ p-Dioxane 0, 0221 5.5 4, 8 0, 09 1, 53 \\ p-Xylene 0, 0311 2.5 8, 5 0, 09 1, 53 \\ mesitylene 0, 0421 2.5 7, 1 0, 03 1, 57 \\ p-Dioxane 0, 0221 5.5 4, 8 0, 09 1, 53 \\ mesitylene 0, 0425 5, 2, 0, 08 1, 81 \\ mesitylene 0, 0338 2.5 4, 6 0, 03 1, 44 \\ Benzene 0, 0308 2.5 7, 6 0, 00 1, 43 \\ Benzene 0, 0226 2.5 9, 6 0, 12 1, 43 \\ 0, 0408 5.5 6, 2 0, 02 1, 43 \\ 0, 0408 5.5 6, 2 0, 02 1, 43 \\ 0, 0408 5.5 6, 2 0, 02 1, 43 \\ 0, 0408 5.5 6, 0 0, 00 1, 44 \\ Benzene 0, 0308 2.5 7, 6 0, 00 1, 44 \\ Benzene 0, 0308 2.5 7, 6 0, 00 1, 44 \\ Benzene 0, 0308 2.5 7, 0 0, 09 1, 71 \\ mesitylene 0, 0425 5, 7, 0 0, 09 1, 71 \\ mesitylene 0, 0448 2.5 6, 6 0, 00 1, 44 \\ Benzene 0, 0266 2.5 13, 4 0, 08 1, 74 \\ mesitylene 0, 0448 2.5 6, 6 0, 00 1, 74 \\ mesitylene 0, 0448 2.5 6, 6 0, 00 1, 74 \\ mesitylene 0, 0448 2.5 7, 7 0, 06 1, 15 \\ p-Xylene 0, 0448 2.5 7, 7 0, 06 1, 15 \\ p-Xylene 0, $	Constations	1,1	-Dicnioro		0.02	1.05
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Dennerane	0.0234	25	2.7	0.02	1.93
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	n Yulana	0.0251	25	4.2	0.00	1.00
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	<i>p</i> -Aylene Mositulono	0.0203	25	4.5	0.02	1.09
$\begin{array}{c} \text{Cyclohexane} & \text{Cyclohexane} & \text{O}, 0463 & 20 & 2.1 & 0.10 & 1.46 \\ \text{Benzene} & 0.0389 & 20 & 3.5 & 0.06 & 1.44 \\ \text{O}, 0389 & 20 & 3.5 & 0.13 & 1.83 \\ \text{O}, 00389 & 50 & 2.9 & 0.03 & 1.76 \\ \text{O}, 0560 & 25 & 4.5 & 0.07 & 1.58 \\ \text{O}, 0560 & 25 & 4.5 & 0.07 & 1.58 \\ \text{O}, 0560 & 25 & 4.5 & 0.07 & 1.58 \\ \text{O}, 0560 & 25 & 4.5 & 0.07 & 1.58 \\ \text{O}, 0560 & 25 & 4.5 & 0.09 & 1.51 \\ \text{O}, 0643 & 25 & 5.3 & 0.08 & 1.51 \\ \text{O}, 0643 & 25 & 5.3 & 0.08 & 1.51 \\ \text{O}, 0643 & 55 & 4.0 & 0.09 & 1.51 \\ \text{P}-Dioxane & 0.0334 & 20 & 6.9 & 0.08 & 1.82 \\ \text{O}, 0232 & 25 & 5.9 & 0.07 & 1.88 \\ \text{O}, 0234 & 25 & 2.9 & 0.02 & 1.84 \\ \text{O}, 0234 & 25 & 2.1 & 0.06 & 1.87 \\ \text{O}, 0275 & 25 & 3.7 & 0.03 & 1.82 \\ \text{P}-Xylene & 0.0275 & 55 & 2.8 & 0.03 & 1.82 \\ \text{P}-Xylene & 0.0417 & 55 & 2.7 & 0.06 & 1.87 \\ \text{Mesitylene} & 0.0495 & 55 & 3.2 & 0.08 & 1.81 \\ \text{P}-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.87 \\ \textbf{Mesitylene} & 0.0495 & 55 & 3.2 & 0.08 & 1.81 \\ \text{P}-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.87 \\ \textbf{Mesitylene} & 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ \text{O}, 0314 & 25 & 3.2 & 0.00 & 1.43 \\ \text{Benzene} & 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ \text{D}-Vxlene & 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ \text{O}, 0311 & 25 & 8.5 & 0.09 & 1.50 \\ \text{O}, 0316 & 55 & 5.6 & 0.08 & 1.49 \\ \text{P}-Dioxane & 0.0328 & 25 & 4.6 & 0.03 & 1.44 \\ \text{Benzene} & 0.0338 & 55 & 3.7 & 0.00 & 1.44 \\ \text{Benzene} & 0.0338 & 55 & 3.7 & 0.00 & 1.44 \\ \text{Benzene} & 0.0346 & 25 & 9.6 & 0.02 & 1.43 \\ \text{D}, Dioxane & 0.0358 & 55 & 3.7 & 0.00 & 1.44 \\ \text{Benzene} & 0.0368 & 25 & 7.6 & 0.00 & 1.44 \\ \text{Benzene} & 0.0266 & 25 & 13.4 & 0.08 & 1.74 \\ \text{O}, 0048 & 55 & 6.2 & 0.02 & 1.43 \\ \text{D}, 0.0266 & 25 & 13.4 & 0.08 & 1.74 \\ \text{Mesitylene} & 0.0448 & 25 & 6.6 & 0.00 & 1.43 \\ \text{Benzene} & 0.0248 & 25 & 6.6 & 0.00 & 1.43 \\ \text{D}, Dioxane & 0.0248 & 25 & 6.6 & 0.00 & 1.43 \\ \text{D}, Dioxane & 0.0248 & 25 & 6.6 & 0.00 & 1.43 \\ \text{D}, Dioxane & 0.0248 & 25 & 6.6 & 0.00 & 1.71 \\ \text{Mesitylene} & 0.0448 & 25 & 6.6 & 0.00 & 1.63 \\ \text{P}-Xylene & 0.0448 & 25 & 8.5 & 0.02 & 1.43 \\ \text{Mesitylene} & 0.0425 & 5$	n Dievene	0.0292	25	4./	0.07	1.91
$\begin{array}{c} Cyclohexane & 0.0463 & 20 & 2.1 & 0.10 & 1.46 \\ 0.0423 & 55 & 1.6 & 0.06 & 1.44 \\ 0.0389 & 20 & 3.5 & 0.13 & 1.83 \\ 0.0389 & 50 & 2.9 & 0.03 & 1.76 \\ p-Xylene & 0.0560 & 25 & 4.5 & 0.07 & 1.58 \\ 0.0560 & 25 & 4.5 & 0.07 & 1.58 \\ 0.0560 & 25 & 4.5 & 0.07 & 1.58 \\ 0.0643 & 20 & 5.8 & 0.08 & 1.49 \\ 0.0643 & 25 & 5.3 & 0.08 & 1.49 \\ 0.0643 & 25 & 5.3 & 0.08 & 1.49 \\ 0.0643 & 25 & 5.9 & 0.07 & 1.88 \\ 1.11-Trichloroethane \\ Cyclohexane & 0.0294 & 25 & 2.9 & 0.02 & 1.84 \\ 0.0294 & 55 & 2.1 & 0.06 & 1.87 \\ Benzene & 0.0275 & 25 & 3.7 & 0.03 & 1.82 \\ p-Xylene & 0.0417 & 25 & 4.0 & 0.07 & 1.76 \\ 0.0475 & 55 & 3.2 & 0.08 & 1.81 \\ p-Dioxane & 0.0294 & 55 & 2.7 & 0.06 & 1.85 \\ Mesitylene & 0.0417 & 25 & 4.0 & 0.07 & 1.76 \\ 0.0495 & 25 & 4.8 & 0.07 & 1.77 \\ p-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.87 \\ p-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.81 \\ p-Dioxane & 0.0211 & 25 & 4.8 & 0.07 & 1.77 \\ p-Dioxane & 0.0211 & 25 & 5.8 & 0.06 & 1.81 \\ p-Dioxane & 0.0211 & 25 & 5.8 & 0.06 & 1.81 \\ p-Dioxane & 0.02121 & 25 & 7.1 & 0.03 & 1.57 \\ p-Xylene & 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ 0.0314 & 55 & 3.2 & 0.08 & 1.81 \\ p-Dioxane & 0.0221 & 25 & 7.6 & 0.02 & 1.43 \\ 0.0326 & 25 & 9.6 & 0.12 & 1.69 \\ 1.1,12-Trictholroethane \\ Cyclohexane & 0.0326 & 25 & 9.6 & 0.12 & 1.69 \\ 1.1,12-Tertachloroethane \\ Cyclohexane & 0.0326 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.02 & 1.43 \\ p-Dioxane & 0.0248 & 55 & 5.0 & 0.00 & 1.44 \\ Benzene & 0.0308 & 55 & 5.2 & 0.00 & 1.45 \\ p-Xylene & 0.0308 & 55 & 5.2 & 0.00 & 1.45 \\ p-Xylene & 0.0408 & 25 & 8.5 & 0.02 & 1.43 \\ 0.0479 & 55 & 7.3 & 0.03 & 1.43 \\ p-Dioxane & 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ p-Xylene & 0.0248 & 55 & 4.0 & 0.09 & 1.71 \\ p-Xylene & 0.0266 & 25 & 13.4 & 0.08 & 1.71 \\ mesitylene & 0.0479 & 25 & 1.7 & 0.08 & 1.63 \\ p-Dioxane & 0.0425 & 55 & 7.7 & 0.06 & 1.55 \\ p-Xylene & 0.0367 & 55 & 7.7 & 0.06 & 1.51 \\ p-Xylene & 0.0367 & 55 & 7.$	p-Dioxane	0.0228	-Dichloro	J.o ethane	0.02	1.98
$\begin{array}{c} 0.0423 55 1.6 0.06 1.44\\ Benzene & 0.0389 50 2.9 0.03 1.76 \\ p-Xylene & 0.0560 20 4.8 0.05 1.58 \\ 0.0560 25 4.5 0.07 1.58 \\ 0.0560 55 3.3 0.09 1.51 \\ 0.0643 25 5.3 0.08 1.49 \\ 0.0643 25 5.3 0.08 1.49 \\ 0.0643 25 5.3 0.08 1.51 \\ 0.0643 55 4.0 0.09 1.51 \\ p-Dioxane 0.0334 20 6.9 0.08 1.82 \\ 0.0232 25 5.9 0.07 1.88 \\ 1.1.1-Trichloroethane \\ Cyclohexane 0.0294 25 2.9 0.02 1.84 \\ 0.0275 25 3.7 0.03 1.82 \\ p-Xylene 0.0417 25 4.0 0.07 1.76 \\ 0.0417 25 4.0 0.07 1.76 \\ 0.0495 55 3.2 0.08 1.81 \\ p-Dioxane 0.0291 25 5.8 0.06 1.87 \\ Benzene 0.0275 25 3.7 0.03 1.82 \\ p-Xylene 0.0417 25 4.0 0.07 1.76 \\ 0.0495 55 3.2 0.08 1.81 \\ p-Dioxane 0.0291 25 5.8 0.06 1.87 \\ I.1.2-Trichloroethane \\ Cyclohexane 0.0314 25 4.1 0.00 1.42 \\ 0.0314 55 3.2 0.08 1.81 \\ p-Dioxane 0.0221 25 5.8 0.06 1.87 \\ I.1.2-Trichloroethane \\ Cyclohexane 0.0311 25 8.5 0.09 1.50 \\ 0.0311 55 5.2 0.08 1.51 \\ Mesitylene 0.0311 25 8.5 0.09 1.50 \\ 0.0311 55 5.6 0.02 1.43 \\ 0.0346 55 5.6 0.08 1.49 \\ p-Dioxane 0.0226 25 9.6 0.02 1.43 \\ 0.0346 55 5.6 0.08 1.49 \\ p-Dioxane 0.0226 25 9.6 0.02 1.43 \\ 0.0346 55 5.2 0.00 1.44 \\ Benzene 0.0358 55 5.2 0.00 1.44 \\ Benzene 0.0308 55 5.2 0.00 1.44 \\ Benzene 0.0308 55 5.2 0.00 1.44 \\ Benzene 0.0378 25 7.6 0.00 1.46 \\ p-Xylene 0.0479 55 7.3 0.03 1.43 \\ p-Dioxane 0.0257 25 13.7 0.04 1.51 \\ Mesitylene 0.0479 55 7.3 0.03 1.43 \\ p-Dioxane 0.0257 25 13.7 0.04 1.71 \\ Mesitylene 0.0266 55 8.0 0.12 1.43 \\ 0.0479 55 7.3 0.03 1.43 \\ p-Dioxane 0.0248 55 4.9 0.09 1.71 \\ Mesitylene 0.0266 55 13.4 0.08 1.74 \\ 0.0368 55 5.9 0.08 1.13 \\ Mesitylene 0.0489 55 4.9 0.00 1.71 \\ Mesitylene 0.0489 55 4.9 0.00 1.71 \\ M$	Cyclobexane	0.0463	20	2.1	0.10	1.46
Benzene 0.0389 20 3.5 0.13 1.83 p -Xylene 0.0389 50 2.9 0.03 1.76 p -Xylene 0.0560 25 4.5 0.07 1.58 0.0560 25 4.5 0.07 1.58 0.0643 20 5.8 0.08 1.41 0.0643 20 5.9 0.07 1.88 p -Dioxane 0.0334 20 6.9 0.08 1.82 p -Dioxane 0.0275 25 2.9 0.07 1.88 p -Xylene 0.0275 25 2.7 0.06 1.87 p -Xylene 0.0417 25 4.0 0.07 1.76 0.0275 55 2.8 0.03 1.82 p -Xylene 0.0495 25 4.8 0.07 1.77 0.0495 25 4.8 0.07 1.76 p -Dioxane 0.0211 25 5.8 0.06 1.87 <	Cyclonexane	0.0423	55	16	0.06	1 44
Definition0.0389502.90.031.76 p -Xylene0.0560204.80.051.580.0560254.50.071.580.0560253.30.091.58Mesitylene0.0643255.30.081.490.0643255.30.081.51 p -Dioxane0.0232255.90.071.88 p -Dioxane0.0294252.90.021.840.0294252.10.061.87Benzene0.0275253.70.031.82 p -Xylene0.0417254.00.071.76Mesitylene0.0495553.20.061.87 p -Dioxane0.0291255.80.061.87 p -Dioxane0.0291255.80.061.87 p -Dioxane0.0211254.10.001.42 p -Dioxane0.021257.10.031.57 p -Dioxane0.0211254.80.091.53 p -Dioxane0.0311258.50.021.43 p -Dioxane0.0311258.50.021.43 p -Dioxane0.0358254.60.031.44 p -Dioxane0.03585.20.001.43 p -Dioxane0.0247251.70.001.45 p -Xylene0.0308257.60.021.43	Benzene	0.0389	20	3.5	0.13	1.83
p-Xylene 0.0560 20 4.8 0.05 1.58 0.0560 25 4.5 0.07 1.58 Mesitylene 0.0643 20 5.8 0.08 1.49 0.0643 25 5.3 0.08 1.51 0.0643 25 5.9 0.07 1.88 0.0232 25 5.9 0.07 1.88 0.0232 25 5.9 0.07 1.88 0.0275 25 2.9 0.02 1.84 0.0275 55 2.8 0.03 1.82 p-Xylene 0.0417 25 4.0 0.07 1.76 0.0495 25 4.8 0.07 1.77 0.0495 25 3.8 0.06 1.87 p-Dioxane 0.021 25 7.8 0.06 1.87 p-Dioxane 0.021 25 7.1 0.03 1.57 p-Xylene 0.0314 25 4.1 0.00 <td></td> <td>0.0389</td> <td>50</td> <td>2.9</td> <td>0.03</td> <td>1.76</td>		0.0389	50	2.9	0.03	1.76
$\begin{array}{c} 0.0560 25 4.5 \\ 0.0560 25 4.5 \\ 0.0560 55 3.3 \\ 0.09 1.58 \\ 0.0643 25 5.3 \\ 0.08 1.49 \\ 0.0643 25 5.3 \\ 0.08 1.49 \\ 0.0643 25 5.3 \\ 0.09 1.51 \\ p-Dioxane \\ 0.0232 25 5.9 \\ 0.07 1.88 \\ 1.1.1-Trichloroethame \\ Cyclohexane \\ 0.0294 25 2.9 \\ 0.0224 25 2.9 \\ 0.021 25 \\ 2.9 \\ 0.0275 55 2.8 \\ 0.03 1.82 \\ 0.0275 55 2.8 \\ 0.03 1.82 \\ p-Xylene \\ 0.0417 25 4.0 \\ 0.077 55 2.8 \\ 0.06 1.87 \\ Mesitylene \\ 0.0495 25 4.8 \\ 0.06 1.87 \\ 0.0495 55 3.2 \\ 0.06 1.87 \\ 0.0495 55 3.2 \\ 0.06 1.87 \\ 0.0495 55 3.2 \\ 0.06 1.87 \\ 0.0495 55 3.2 \\ 0.06 1.87 \\ 0.0495 55 3.2 \\ 0.06 1.87 \\ 0.0495 55 3.2 \\ 0.06 1.87 \\ 0.0314 55 3.2 \\ 0.06 1.87 \\ 0.0314 55 3.2 \\ 0.00 1.43 \\ Benzene \\ 0.0221 25 5.8 \\ 0.06 1.87 \\ 0.0221 25 4.8 \\ 0.09 1.53 \\ p-Xylene \\ 0.0314 25 4.1 \\ 0.03 1.57 \\ 0.0221 55 4.8 \\ 0.09 1.53 \\ p-Xylene \\ 0.0311 25 8.5 \\ 0.09 1.50 \\ 0.0311 55 5.2 \\ 0.08 1.51 \\ Mesitylene \\ 0.0346 55 5.6 \\ 0.08 1.43 \\ p-Dioxane \\ 0.0226 25 9.6 \\ 0.12 1.69 \\ 1.1,1.2-Tetrachloroethame \\ Cyclohexane \\ 0.0358 55 3.7 \\ 0.00 1.44 \\ Benzene \\ 0.0308 55 5.2 \\ 0.00 1.45 \\ p-Xylene \\ 0.0308 55 5.7 \\ 0.00 1.45 \\ p-Xylene \\ 0.0308 55 5.7 \\ 0.00 1.45 \\ p-Xylene \\ 0.0248 25 8.5 \\ 0.02 1.43 \\ 0.0408 25 8.5 \\ 0.02 1.43 \\ 0.0408 55 6.2 \\ 0.02 1.43 \\ 0.0408 55 6.2 \\ 0.02 1.43 \\ p-Dioxane \\ 0.0257 25 13.7 \\ 0.04 1.53 \\ 1.1,2.2-Tetrachloroethame \\ Cyclohexane \\ 0.0248 55 6.0 \\ 0.0248 55 7.0 \\ 0.09 1.71 \\ 0.0213 55 7.0 \\ 0.09 1.71 \\ 0.0213 55 7.0 \\ 0.09 1.71 \\ 0.0266 55 8.0 \\ 0.012 1.71 \\ 0.0428 55 6.0 \\ 0.00 1.60 \\ Benzene \\ 0.0248 55 6.0 \\ 0.0248 55 6.0 \\ 0.00 1.71 \\ 0.0266 55 8.0 \\ 0.012 1.71 \\ 0.0587 59 7.0 \\ 0.08 1.71 \\ 0.0425 55 7.7 \\ 0.06 1.71 \\ 0.0425 55 7.7 \\ 0.06 1.71 \\ 0.0425 55 7.7 \\ 0.06 1.71 \\ 0.0425 55 7.7 \\ 0.06 1.71 \\ 0.0425 55 7.7 \\ 0.06 1.71 \\ $	<i>p</i> -Xylene	0.0560	20	4.8	0.05	1.58
Mesitylene 0.0560 55 3.3 0.09 1.58 Mesitylene 0.0643 20 5.8 0.08 1.49 0.0643 25 5.3 0.08 1.51 p -Dioxane 0.0334 20 6.9 0.08 1.82 0.0232 25 5.9 0.07 1.88 $1,1,1$ -Trichloroethane 0.0294 25 2.9 0.02 1.84 Benzene 0.0275 25 3.7 0.03 1.82 p -Xylene 0.0417 25 4.0 0.07 1.76 0.0417 25 4.0 0.07 1.76 0.0495 55 3.2 0.08 1.81 p -Xylene 0.0291 25 5.8 0.06 1.87 p -Dioxane 0.021 25 7.1 0.03 1.57 p -Xylene 0.0314 25 4.6 0.02 1.43 0.0346 25 9.6 0.02 1.43 p -Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,2$ -Tetrachloroethane $1.1,2-7$ 1.42 1.49 p -Dioxane 0.0226 25 9.6 0.02 1.43 p -Dioxane 0.0262 25 6.6 0.00 1	1 ,	0.0560	25	4.5	0.07	1.58
Mesitylene 0.0643 20 5.8 0.08 1.49 0.0643 25 5.3 0.08 1.51 p -Dioxane 0.0334 20 6.9 0.08 1.82 0.0232 25 5.9 0.07 1.88 $1,1,1$ -Trichloroethane 0.0294 25 2.9 0.02 1.84 0.0275 25 3.7 0.03 1.82 0.0275 55 2.8 0.03 1.82 p -Xylene 0.0417 25 4.0 0.07 1.76 0.0275 55 3.2 0.08 1.81 p -Dioxane 0.0291 25 5.8 0.06 1.87 p -Dioxane 0.0211 25 7.1 0.03 1.51 p -Dioxane 0.0311 25 5.2 0.08 1.81 p -Zylene 0.0311 25 5.2 0.08 1.51 Mesitylene 0.0346 25 9.6<		0.0560	55	3.3	0.09	1.58
$\begin{array}{c} 0.0643 & 25 & 5.3 & 0.08 & 1.51 \\ 0.0643 & 55 & 4.0 & 0.09 & 1.51 \\ 0.0334 & 20 & 6.9 & 0.08 & 1.82 \\ 0.0232 & 25 & 5.9 & 0.07 & 1.88 \\ 1.1.1-Trichloroethane \\ Cyclohexane & 0.0294 & 25 & 2.9 & 0.02 & 1.84 \\ 0.0294 & 25 & 2.1 & 0.06 & 1.87 \\ Benzene & 0.0275 & 25 & 3.7 & 0.03 & 1.82 \\ 0.0275 & 55 & 2.8 & 0.03 & 1.82 \\ 0.0417 & 25 & 4.0 & 0.07 & 1.76 \\ 0.0417 & 25 & 4.0 & 0.07 & 1.76 \\ 0.0417 & 55 & 2.7 & 0.06 & 1.85 \\ Mesitylene & 0.0495 & 25 & 4.8 & 0.07 & 1.77 \\ 0.0495 & 55 & 3.2 & 0.08 & 1.81 \\ p-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.87 \\ 1.1.2-Trichloroethane \\ Cyclohexane & 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ 0.0314 & 25 & 4.1 & 0.00 & 1.43 \\ Benzene & 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0211 & 25 & 8.5 & 0.09 & 1.53 \\ p-Xylene & 0.0311 & 25 & 8.5 & 0.09 & 1.53 \\ p-Lioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ 1.1,1.2-Tetrachloroethane \\ Cyclohexane & 0.0328 & 25 & 4.6 & 0.03 & 1.44 \\ p-Dioxane & 0.0328 & 25 & 4.6 & 0.03 & 1.44 \\ p-Dioxane & 0.0388 & 55 & 3.7 & 0.00 & 1.44 \\ Benzene & 0.0308 & 25 & 7.6 & 0.00 & 1.45 \\ p-Xylene & 0.0408 & 25 & 8.5 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ p-Dioxane & 0.0257 & 25 & 13.7 & 0.04 & 1.53 \\ p-Xylene & 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ p-Dioxane & 0.0213 & 25 & 10.4 & 0.12 & 1.43 \\ p-Dioxane & 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 55 & 4.0 & 0.09 & 1.71 \\ mesitylene & 0.0408 & 55 & 6.2 & 0.02 & 1.41 \\ Mesitylene & 0.0408 & 55 & 6.2 & 0.02 & 1.41 \\ Mesitylene & 0.0248 & 55 & 6.0 & 0.01 & 1.65 \\ 0.0300 & 55 & 11.7 & 0.08 & 1.77 \\ p-Xylene & 0.0266 & 25 & 13.4 & 0.08 & 1.77 \\ mesitylene & 0.0248 & 55 & 4.9 & 0.00 & 1.63 \\ p-Dioxane & 0.0248 & 55 & 4.9 & 0.00 & 1.63 \\ p-Dioxane & 0.0248 & 55 & 4.9 & 0.00 & 1.63 \\ p-Dioxane & 0.0248 & 55 & 12.7 & 0.08 & 1.77 \\ mesitylene & 0.0300 & 55 & 11.7 & 0.08 & 1.63 \\ p-Dioxane & 0.0489 & 55 & 4.9 & 0.00 & 1.63 \\ p-Xylene & 0.0674 & 25 & 12.7 & 0.08 & 1.17 \\ mostrylene & 0.0674 & 25 & 12.7 & 0.08 & 1.13 \\ Mesitylene & 0.0674 & 25 & 27.6 & 0.08 & $	Mesitylene	0.0643	20	5.8	0.08	1.49
$\begin{array}{c cccccc} 0.0643 & 55 & 4.0 & 0.09 & 1.51 \\ 0.0334 & 20 & 6.9 & 0.08 & 1.82 \\ 0.0232 & 25 & 5.9 & 0.07 & 1.88 \\ 1,1,1-Trichloroethane \\ \hline Cyclohexane & 0.0294 & 25 & 2.9 & 0.02 & 1.84 \\ 0.0275 & 25 & 3.7 & 0.03 & 1.82 \\ 0.0275 & 55 & 2.8 & 0.03 & 1.82 \\ p-Xylene & 0.0417 & 25 & 4.0 & 0.07 & 1.76 \\ 0.0417 & 25 & 4.0 & 0.07 & 1.77 \\ 0.0495 & 25 & 3.2 & 0.08 & 1.81 \\ p-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.87 \\ \hline P-Dioxane & 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ 0.0314 & 25 & 4.1 & 0.00 & 1.43 \\ Benzene & 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 25 & 7.4 & 8 & 0.09 & 1.53 \\ p-Xylene & 0.0311 & 25 & 8.5 & 0.09 & 1.53 \\ p-Xylene & 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ 0.0308 & 55 & 5.2 & 0.08 & 1.43 \\ 0.0366 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0358 & 55 & 3.7 & 0.00 & 1.44 \\ Benzene & 0.0308 & 55 & 5.2 & 0.00 & 1.45 \\ p-Xylene & 0.0408 & 25 & 8.5 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ p-Dioxane & 0.0257 & 25 & 13.7 & 0.04 & 1.53 \\ p-Xylene & 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ p-Xylene & 0.0248 & 55 & 4.0 & 0.09 & 1.60 \\ Benzene & 0.0213 & 25 & 10.4 & 0.12 & 1.43 \\ p-Dioxane & 0.0248 & 55 & 6.0 & 0.12 & 1.71 \\ Mesitylene & 0.0479 & 55 & 7.3 & 0.03 & 1.43 \\ p-Dioxane & 0.0248 & 55 & 4.0 & 0.09 & 1.71 \\ p-Xylene & 0.0266 & 25 & 13.4 & 0.08 & 1.77 \\ 0.0489 & 55 & 4.9 & 0.00 & 1.63 \\ p-Xylene & 0.0648 & 55 & 6.0 & 0.01 & 1.71 \\ P-Xylene & 0.0668 & 25 & 15.4 & 0.08 & 1.77 \\ 0.0425 & 55 & 7.7 & 0.06 & 1.59 \\ P-Xylene & 0.0674 & 25 & 15.7 & 0.08 & 1.63 \\ p-Xylene & 0.0489 & 55 & 4.9 & 0.00 & 1.63 \\ P-Dioxane & 0.0489 & 55 & 6.0 & 0.00 & 1.88 \\ \hline Pentachloroethane \\ \hline P-Xylene & 0.0674 & 25 & 15.7 & 0.08 & 1.13 \\ \hline Mesitylene & 0.0674 & 55 & 15.7$	•	0.0643	25	5.3	0.08	1.51
p-Dioxane 0.0334 20 6.9 0.08 1.82 0.0232 25 5.9 0.07 1.88 1,1,1-Trichloroethane 0.0294 25 2.9 0.02 1.84 Benzene 0.0275 25 3.7 0.03 1.82 p -Xylene 0.0417 25 4.0 0.07 1.76 0.0417 25 4.8 0.07 1.77 0.0495 25 4.8 0.07 1.77 0.0495 25 3.7 0.06 1.87 p-Dioxane 0.0291 25 5.8 0.06 1.87 p-Dioxane 0.021 25 5.8 0.06 1.87 p-Dioxane 0.0221 25 4.8 0.09 1.53 p-Xylene 0.0311 25 8.5 0.09 1.53 p-Zylene 0.0326 25 9.6 0.12 1.69 p-Dioxane 0.0226 25 9.6 0.12		0.0643	55	4.0	0.09	1.51
0.0232 25 5.9 0.07 1.88 $1,1,1$ -Trichloroethane 0.0294 25 2.9 0.02 1.84 0.0294 25 2.1 0.06 1.87 Benzene 0.0275 25 3.7 0.03 1.82 p -Xylene 0.0417 25 4.8 0.07 1.76 0.0417 25 4.8 0.07 1.77 0.0495 25 4.8 0.07 1.77 0.0495 25 4.8 0.07 1.43 p -Dioxane 0.0291 25 5.8 0.06 1.87 p -Dioxane 0.0221 25 7.1 0.03 1.57 p -Xylene 0.0311 25 8.5 0.09 1.50 p -Xylene 0.0346 25 9.6 0.12 1.69 p -Xylene 0.0368 25 7.6 0.02 1.43	p-Dioxane	0.0334	20	6.9	0.08	1.82
$\begin{array}{c c} 1,1,1-Trichloroethane \\ 0.0294 25 2.9 0.02 \\ 1.84 \\ 0.0275 25 3.7 0.03 1.82 \\ 0.0275 55 2.8 0.03 1.82 \\ 0.0275 55 2.8 0.03 1.82 \\ 0.0417 25 4.0 0.07 1.76 \\ 0.0417 25 4.0 0.07 1.76 \\ 0.0417 55 2.7 0.06 1.85 \\ Mesitylene 0.0495 25 4.8 0.07 1.77 \\ 0.0495 55 3.2 0.08 1.81 \\ p-Dioxane 0.0291 25 5.8 0.06 1.87 \\ 1,1,2-Trichloroethane \\ Cyclohexane 0.0314 25 4.1 0.00 1.42 \\ 0.0314 55 3.2 0.00 1.43 \\ 0.0314 55 3.2 0.00 1.43 \\ 0.0314 55 3.2 0.00 1.43 \\ 0.0311 55 5.2 0.08 1.51 \\ 0.0221 25 7.1 0.03 1.57 \\ 0.0221 25 7.1 0.03 1.57 \\ 0.0221 25 5.6 0.02 1.43 \\ 0.0346 55 5.6 0.09 1.50 \\ 0.0311 55 5.2 0.08 1.51 \\ Mesitylene 0.0346 55 5.6 0.08 1.49 \\ p-Dioxane 0.0226 25 9.6 0.12 1.69 \\ p-Dioxane 0.0226 25 9.6 0.12 1.69 \\ p-Dioxane 0.0368 55 3.7 0.00 1.44 \\ 0.0358 55 3.7 0.00 1.44 \\ 0.0388 55 3.7 0.00 1.44 \\ 0.0388 55 5.2 0.00 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0408 55 6.2 0.00 1.45 \\ p-Xylene 0.0408 25 8.5 0.02 1.43 \\ 0.0408 55 6.2 0.02 1.43 \\ 0.0415 55 7.0 0.09 1.60 \\ 0.0248 25 5.6 0.06 1.59 \\ 0.0248 55 4.0 0.09 1.60 \\ 0.0248 55 4.0 0.09 1.60 \\ 0.0266 55 8.0 0.12 1.71 \\ 0.0266 55 8.0 0.12 1.71 \\ 0.0266 55 8.0 0.12 1.71 \\ 0.048 55 4.9 0.00 1.03 \\ 0.048 55 4.9 0.00 1.03 \\ 0.048 55 4.9 0.00 1.03 \\ 0.048 55 4.9 0.00 1.03 \\ 0.0425 55 7.7 0.06 1.57 \\ 0.048 55 4.9 0.00 1.03 \\ 0.0674 55 1$	-	0.0232	25	5.9	0.07	1.88
$\begin{array}{c} Cyclohexane & 0.0294 & 25 & 2.9 & 0.02 & 1.84 \\ 0.0294 & 55 & 2.1 & 0.06 & 1.87 \\ Benzene & 0.0275 & 25 & 3.7 & 0.03 & 1.82 \\ 0.0275 & 55 & 2.8 & 0.03 & 1.82 \\ p-Xylene & 0.0417 & 25 & 4.0 & 0.07 & 1.76 \\ 0.0417 & 25 & 4.0 & 0.07 & 1.77 \\ 0.0495 & 55 & 3.2 & 0.08 & 1.81 \\ p-Dioxane & 0.0291 & 25 & 5.8 & 0.06 & 1.87 \\ \hline \\ Delioxane & 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ 0.0314 & 55 & 3.2 & 0.00 & 1.43 \\ Benzene & 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 25 & 8.5 & 0.09 & 1.50 \\ p-Xylene & 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ 0.0346 & 55 & 5.6 & 0.08 & 1.49 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ p-Dioxane & 0.0258 & 55 & 3.7 & 0.00 & 1.44 \\ Benzene & 0.0308 & 25 & 7.6 & 0.00 & 1.45 \\ p-Xylene & 0.0308 & 25 & 7.6 & 0.00 & 1.45 \\ p-Xylene & 0.0408 & 25 & 8.5 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0479 & 25 & 10.4 & 0.12 & 1.43 \\ 0.0479 & 25 & 10.4 & 0.12 & 1.43 \\ p-Dioxane & 0.0277 & 25 & 13.7 & 0.04 & 1.53 \\ r_1,1,2,2-Tetrachloroethane \\ Cyclohexane & 0.0278 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0266 & 55 & 8.0 & 0.12 & 1.71 \\ Mesitylene & 0.0266 & 25 & 13.4 & 0.08 & 1.74 \\ 0.0266 & 55 & 8.0 & 0.12 & 1.71 \\ Mesitylene & 0.0425 & 25 & 7.7 & 0.08 & 1.63 \\ p-Dioxane & 0.0164 & 25 & 18.6 & 0.00 & 1.88 \\ \hline Pentachloroethane \\ Cyclohexane & 0.0489 & 25 & 6.6 & 0.00 & 1.88 \\ \hline Pentachloroethane \\ Pentachloroethane \\ Cyclohexane & 0.0489 & 25 & 6.6 & 0.00 & 1.60 \\ Benzene & 0.0489 & 25 & 6.6 & 0.00 & 1.61 \\ p-Dioxane & 0.0674 & 25 & 12.7 & 0.08 & 1.63 \\ p-Dioxane & 0.0675 & 25 & 7.6 & 0.08 & 1.13 \\ Mesit$		1,1,1	-Trichloro	oethane		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Cyclohexane	0.0294	25	2.9	0.02	1.84
Benzene 0.0275 25 3.7 0.03 1.82 p -Xylene 0.0417 25 4.0 0.07 1.76 0.0417 25 4.0 0.07 1.77 0.0495 25 4.8 0.07 1.77 p -Dioxane 0.0291 25 5.8 0.06 1.81 p -Dioxane 0.0291 25 5.8 0.06 1.87 $1,1,2$ -Trichloroethane 0.0314 25 4.1 0.00 1.42 0.0314 25 4.1 0.00 1.43 Benzene 0.0221 25 7.1 0.03 1.57 0.0221 25 7.1 0.03 1.57 p -Xylene 0.0311 25 8.5 0.09 1.50 p -Xylene 0.0311 25 8.5 0.09 1.50 p -Dioxane 0.0226 25 9.6 0.12 1.69 p -Dioxane 0.0226 25 9.6 0.12 1.69 p -Dioxane 0.0238 25 7.6 0.00 1.44 p -Dioxane 0.0308 25 7.6 0.00 1.45 p -Xylene 0.0408 25 8.5 0.02 1.41 Mesitylene 0.027 25 13.7 0.04 1.53 p -Xylene 0.0264 25 5.6 0.06 1.59 p -Xylene 0.0264 25 8.6 0.02 1.43 p -Dioxane 0.0213 25 1		0.0294	55	2.1	0.06	1.87
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Benzene	0.0275	25	3.7	0.03	1.82
p-Xylene 0.0417 25 4.0 0.07 1.76 0.0495 25 4.8 0.07 1.77 0.0495 25 4.8 0.07 1.77 0.0495 55 3.2 0.08 1.81 p-Dioxane 0.0291 25 5.8 0.06 1.87 $1.1,2$ -Trichloroethane 0.0314 25 4.1 0.00 1.42 0.0314 25 4.1 0.00 1.43 Benzene 0.0221 25 7.1 0.03 1.57 0.0221 55 4.8 0.09 1.53 p -Xylene 0.0311 25 8.5 0.09 1.50 0.0311 25 8.5 0.09 1.50 0.0346 25 9.6 0.12 1.69 p -Dioxane 0.0226 25 9.6 0.12 1.69 p -Dioxane 0.0358 55 3.7 0.00 1.44 Benzene 0.0308 25 7.6 0.00 1.45 p -Xylene 0.0408 25 8.5 0.02 1.43 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 p -Dioxane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0248 25 6.6 0.00 1.60 Benzene 0.0266 25 13.4 0.08		0.0275	55	2.8	0.03	1.82
0.0417552.7 0.06 1.85 Mesitylene 0.0495 25 4.8 0.07 1.77 0.0495 55 3.2 0.08 1.87 p -Dioxane 0.0291 25 5.8 0.06 1.87 Cyclohexane 0.0314 25 4.1 0.00 1.42 0.0314 25 4.1 0.00 1.42 0.0221 25 7.1 0.03 1.57 p -Xylene 0.0311 25 8.5 0.09 1.50 0.0311 25 8.5 0.09 1.50 0.0346 25 9.6 0.12 1.69 p -Xylene 0.0346 25 9.6 0.12 1.69 0.0346 55 5.2 0.08 1.44 p -Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -Tetrachloroethane $Cyclohexane$ 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.44 p -Xylene 0.0408 25 8.5 0.02 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 p -Xylene 0.0248 25 5.6 0.006 1.59 0.0248 25 6.6 0.00 1.60 Benzene 0.0213 25 10.4 0.05 1.71 p -Xy	<i>p</i> -Xylene	0.0417	25	4.0	0.07	1.76
Mesitylene 0.0495 25 4.8 0.07 1.77 0.0495 55 3.2 0.08 1.81 p -Dioxane 0.0291 25 5.8 0.06 1.87 Cyclohexane 0.0314 25 4.1 0.00 1.42 0.0314 25 4.1 0.00 1.43 Benzene 0.0221 25 7.1 0.03 1.57 0.0221 25 7.1 0.03 1.57 p -Xylene 0.0311 25 8.5 0.09 1.50 0.0311 25 8.5 0.09 1.50 0.0311 25 8.5 0.02 1.43 p -Xylene 0.0346 25 9.6 0.12 1.69 p -Dioxane 0.0226 25 9.6 0.12 1.69 p -Dioxane 0.0226 25 9.6 0.12 1.69 p -Dioxane 0.0226 25 9.6 0.12 1.69 p -Xylene 0.0308 25 7.6 0.00 1.46 p -Xylene 0.0408 25 6.2 0.02 1.43 p -Xylene 0.0408 25 6.2 0.02 1.43 p -Xylene 0.0408 25 6.2 0.02 1.43 p -Xylene 0.0257 25 13.7 0.04 1.53 p -Xylene 0.0248 25 6.6 0.00 1.60 Benzene 0.0213 25 10.4 0.05 1.71		0.0417	55	2.7	0.06	1.85
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mesitylene	0.0495	25	4.8	0.07	1.77
p-Dioxane 0.0291 25 5.8 0.06 1.87 1,1,2-TrichloroethaneCyclohexane 0.0314 25 4.1 0.00 1.42 Benzene 0.0221 25 7.1 0.03 1.57 0.0221 55 4.8 0.09 1.53 p -Xylene 0.0311 25 8.5 0.09 1.50 0.0311 25 8.5 0.09 1.50 0.0316 25 9.6 0.02 1.43 p -Xylene 0.0346 25 9.6 0.02 0.0346 25 9.6 0.12 1.69 0.0346 25 9.6 0.12 1.69 p -Dioxane 0.0226 25 9.6 0.12 0.0378 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 0.308 55 5.2 0.00 1.45 p -Xylene 0.0408 25 8.5 0.02 0.4079 25 10.4 0.12 1.43 0.0408 25 8.5 0.02 1.43 p -Dioxane 0.0257 25 13.7 0.04 $1.1,2,2$ -Tetrachloroethane 0.0248 25 5.6 0.0248 25 5.6 0.06 1.59 p -Dioxane 0.0248 25 5.6 0.06 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0213 25 <td></td> <td>0.0495</td> <td>55</td> <td>3.2</td> <td>0.08</td> <td>1.81</td>		0.0495	55	3.2	0.08	1.81
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	<i>p</i> -Dioxane	0.0291	25	5.8	0.06	1.87
$\begin{array}{c} Cyclohexane & 0.0314 & 25 & 4.1 & 0.00 & 1.42 \\ 0.0314 & 55 & 3.2 & 0.00 & 1.43 \\ Benzene & 0.0221 & 25 & 7.1 & 0.03 & 1.57 \\ 0.0221 & 55 & 4.8 & 0.09 & 1.53 \\ p-Xylene & 0.0311 & 25 & 8.5 & 0.09 & 1.50 \\ 0.0311 & 55 & 5.2 & 0.08 & 1.51 \\ Mesitylene & 0.0346 & 25 & 9.6 & 0.02 & 1.43 \\ 0.0346 & 55 & 5.6 & 0.08 & 1.49 \\ p-Dioxane & 0.0226 & 25 & 9.6 & 0.12 & 1.69 \\ 1,1,1,2-Tetrachloroethane \\ Cyclohexane & 0.0358 & 25 & 4.6 & 0.03 & 1.44 \\ Benzene & 0.0308 & 25 & 7.6 & 0.00 & 1.45 \\ p-Xylene & 0.0408 & 25 & 8.5 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ p-Dioxane & 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.43 \\ p-Dioxane & 0.0257 & 25 & 13.7 & 0.04 & 1.53 \\ 1,1,2.2-Tetrachloroethane \\ Cyclohexane & 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 55 & 4.0 & 0.09 & 1.60 \\ Benzene & 0.0213 & 25 & 10.4 & 0.05 & 1.71 \\ 0.0213 & 55 & 7.0 & 0.09 & 1.60 \\ Benzene & 0.0266 & 55 & 8.0 & 0.12 & 1.71 \\ p-Xylene & 0.0266 & 55 & 8.0 & 0.12 & 1.71 \\ Mesitylene & 0.0300 & 25 & 19.7 & 0.12 & 1.65 \\ 0.0300 & 55 & 11.7 & 0.08 & 1.63 \\ p-Dioxane & 0.0164 & 25 & 18.6 & 0.00 & 1.88 \\ \hline Pentachloroethane \\ Cyclohexane & 0.0489 & 25 & 6.6 & 0.00 & 1.07 \\ 0.0489 & 55 & 4.9 & 0.00 & 1.03 \\ Benzene & 0.0489 & 25 & 6.6 & 0.00 & 1.71 \\ p-Xylene & 0.0587 & 25 & 15.4 & 0.08 & 1.17 \\ 0.0674 & 25 & 15.4 & 0.08 & 1.17 \\ 0.0587 & 55 & 9.5 & 0.08 & 1.13 \\ Mesitylene & 0.0674 & 25 & 21.7 & 0.10 & 1.11 \\ Mesitylene & 0.0674 & 25 & 21.7 & 0.10 & 1.11 \\ 0.0674 & 55 & 16.7 & 0.09 & 1.09 \\ p-Dioxane & 0.0376 & 25 & 27.6 & 0.08 & 1.26 \\ \hline \end{tabular}$		1,1,2	2-Trichlor	oethane		
0.031455 3.2 0.00 1.43 Benzene 0.0221 25 7.1 0.03 1.57 0.0221 55 4.8 0.09 1.53 p -Xylene 0.0311 25 8.5 0.09 1.50 Mesitylene 0.0346 25 9.6 0.02 1.43 0.0346 25 9.6 0.02 1.43 p -Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -Tetrachloroethane $Cyclohexane$ 0.038 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.44 Benzene 0.0308 25 7.6 0.00 1.44 Benzene 0.0308 25 7.6 0.00 1.43 p -Xylene 0.0408 25 6.2 0.02 1.43 0.0408 25 6.2 0.02 1.43 p -Xylene 0.0408 55 6.2 0.02 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 $1,1,2,2$ -Tetrachloroethane $Cyclohexane$ 0.0248 25 6.006 1.59 0.0248 25 4.0 0.09 1.60 Benzene 0.0266 25 13.4 0.08 1.71 p -Xylene 0.0266 25 13.4 0.08 1.71 p -Xylene 0.0266 <td>Cyclohexane</td> <td>0.0314</td> <td>25</td> <td>4.1</td> <td>0.00</td> <td>1.42</td>	Cyclohexane	0.0314	25	4.1	0.00	1.42
Benzene 0.0221 25 7.1 0.03 1.57 p -Xylene 0.0311 25 8.5 0.09 1.50 0.0311 55 5.2 0.08 1.51 Mesitylene 0.0346 25 9.6 0.022 1.43 p -Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -Tetrachloroethane 1.44 0.0358 25 4.6 0.03 1.44 Benzene 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.46 p -Xylene 0.0408 25 8.5 0.02 1.43 p -Xylene 0.0408 25 8.5 0.02 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 p -Dioxane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0248 25 10.4 0.05 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0266 25 13.4 0.08 1.74 0.0266 55 8.0 0.12 1.71 p -Xylene 0.0300 25 19.7 0.12 1.65 p -Dioxane 0.0164 25 18.6 0.00 1.03 p -Dioxane 0.0164 25 <td< td=""><td>_</td><td>0.0314</td><td>55</td><td>3.2</td><td>0.00</td><td>1.43</td></td<>	_	0.0314	55	3.2	0.00	1.43
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Benzene	0.0221	25	7.1	0.03	1.57
p-Xylene 0.0311 25 8.5 0.09 1.50 Mesitylene 0.0346 25 9.6 0.02 1.43 0.0346 55 5.6 0.08 1.49 p-Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -Tetrachloroethane 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.44 Benzene 0.0308 25 8.5 0.02 1.43 p -Xylene 0.0408 25 8.5 0.02 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0248 25 5.6 0.06 1.59 p -Dioxane 0.0248 25 5.6 0.06 1.59 p -Xylene 0.0266		0.0221	55	4.8	0.09	1.53
0.0311 55 5.2 0.08 1.51 Mesitylene 0.0346 25 9.6 0.02 1.43 0.0346 55 5.6 0.08 1.49 p -Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -Tetrachloroethane $1.1,1,2$ -TetrachloroethaneCyclohexane 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.44 Benzene 0.0308 25 8.5 0.02 1.43 p -Xylene 0.0408 25 8.5 0.02 1.43 0.0408 25 6.2 0.02 1.43 0.0408 25 6.2 0.02 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 $1,1,2,2$ -Tetrachloroethane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0266 55 8.0 0.12 1.71 p -Xylene 0.0266 55 8.0 0.12 1.71 p -Xylene 0.0266 55 8.0 0.12 1.71 p -Xylene 0.0489 25 </td <td><i>p</i>-Xylene</td> <td>0.0311</td> <td>25</td> <td>8.5</td> <td>0.09</td> <td>1.50</td>	<i>p</i> -Xylene	0.0311	25	8.5	0.09	1.50
Mesntylene 0.0346 25 9.6 0.02 1.43 p -Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -TetrachloroethaneCyclohexane 0.0358 25 4.6 0.03 1.44 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.44 Benzene 0.0308 25 7.6 0.00 1.44 p -Xylene 0.0408 25 8.5 0.02 1.43 0.0408 55 6.2 0.02 1.43 0.0408 55 6.2 0.02 1.41 Mesitylene 0.0479 25 10.4 0.12 1.43 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 $1,1,2,2$ -Tetrachloroethane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0213 25 10.4 0.05 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0300 25 19.7 0.12 1.63 p -Dioxane 0.0164 25 18.6 0.00 1.03 p -Dioxane 0.0674 25 12.7 0.08 1.07 0.0425 55 7.7 0.06 1.17 p -Dioxane 0.0489 25 6.6 0.00 </td <td></td> <td>0.0311</td> <td>55</td> <td>5.2</td> <td>0.08</td> <td>1.51</td>		0.0311	55	5.2	0.08	1.51
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mesitylene	0.0346	25	9.6	0.02	1.43
p-Dioxane 0.0226 25 9.6 0.12 1.69 $1,1,1,2$ -TetrachloroethaneCyclohexane 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 25 7.6 0.00 1.46 0.0308 25 7.6 0.00 1.45 p -Xylene 0.0408 25 8.5 0.02 1.43 0.0408 25 8.5 0.02 1.43 p -Xylene 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 p -Dioxane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0213 25 10.4 0.05 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0266 55 8.0 0.12 1.71 p -Xylene 0.0164 25 18.6 0.00 1.88 p -Dioxane 0.0164 25 18.6 0.00 1.03 p -Dioxane 0.0489 25 6.6 0.00 1.07 0.0425 25 7.7 0.08 1.07 p -Dioxane 0.0425 25 7.7 0.08 1.07 p -Dioxane 0.0425 25 12.7 0.08 1.17 p -Dioxane 0.0425 25 12.7 0		0.0346	22	5.6	0.08	1.49
$\begin{array}{c} \mbox{Lightarred} 1,1,1,2-1 \mbox{etrachloroethane} \\ \mbox{Cyclohexane} & 0.0358 & 25 & 4.6 & 0.03 & 1.44 \\ \mbox{Benzene} & 0.0308 & 25 & 7.6 & 0.00 & 1.46 \\ 0.0308 & 55 & 5.2 & 0.00 & 1.45 \\ \mbox{p-Xylene} & 0.0408 & 25 & 8.5 & 0.02 & 1.43 \\ 0.0408 & 55 & 6.2 & 0.02 & 1.41 \\ \mbox{Mesitylene} & 0.0479 & 25 & 10.4 & 0.12 & 1.43 \\ 0.0479 & 55 & 7.3 & 0.03 & 1.43 \\ \mbox{p-Dioxane} & 0.0257 & 25 & 13.7 & 0.04 & 1.53 \\ \mbox{$1,1,2,2$-Tetrachloroethane} \\ \mbox{Cyclohexane} & 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ 0.0213 & 55 & 4.0 & 0.09 & 1.60 \\ \mbox{Benzene} & 0.0266 & 25 & 13.4 & 0.08 & 1.71 \\ \mbox{$0.0266 & 25 & 13.4 & 0.08 & 1.74 \\ 0.0266 & 55 & 8.0 & 0.12 & 1.71 \\ \mbox{$0.0300 & 25 & 19.7 & 0.12 & 1.65 \\ 0.0300 & 55 & 11.7 & 0.08 & 1.63 \\ \mbox{p-Dioxane} & 0.0164 & 25 & 18.6 & 0.00 & 1.88 \\ \mbox{$metachloroethane} \\ \mbox{$Cyclohexane} & 0.0489 & 25 & 6.6 & 0.00 & 1.07 \\ \mbox{$0.0489 & 55 & 4.9 & 0.00 & 1.03 \\ \mbox{$benzene & 0.0425 & 25 & 12.7 & 0.08 & 1.07 \\ \mbox{$0.0425 & 55 & 7.7 & 0.06 & 1.15 \\ \mbox{p-Xylene & 0.0587 & 55 & 9.5 & 0.08 & 1.13 \\ \mbox{$0.0587 & 55 & 9.5 & 0.08 & 1.13 \\ \mbox{$Mesitylene & 0.0674 & 25 & 21.7 & 0.10 & 1.11 \\ \mbox{$0.0674 & 55 & 16.7 & 0.09 & 1.09 \\ \mbox{p-Dioxane & 0.0376 & 25 & 27.6 & 0.08 & 1.26 \\ \end{tabular}$	<i>p</i> -Dioxane	0.0226	25	9.6	0.12	1.69
Cyclonexane 0.0358 25 4.6 0.03 1.44 Benzene 0.0308 55 3.7 0.00 1.46 Benzene 0.0308 25 7.6 0.00 1.45 p -Xylene 0.0408 25 8.5 0.02 1.43 0.0408 25 8.5 0.02 1.43 0.0408 55 6.2 0.02 1.41 Mesitylene 0.0479 25 10.4 0.12 1.43 0.0479 55 7.3 0.03 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 $1,1,2,2$ -Tetrachloroethane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0213 25 10.4 0.05 1.71 0.0213 25 10.4 0.08 1.74 0.0266 25 13.4 0.08 1.74 0.0266 25 13.4 0.08 1.63 p -Dioxane 0.0164 25 18.6 0.00 1.88 Pentachloroethane $Cyclohexane$ 0.0425 25 7.7 0.08 1.07 0.0425 25 12.7 0.08 1.07 0.0425 55 7.7 0.06 1.15 p -Dioxane 0.0674 25 21.7 0.08 1.17 0.08 1.17 p -Xylene 0.0674 25 21.7 0.08 1.13 Me	0	1,1,1,2	-Tetrachic	broethane	0.02	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cyclohexane	0.0358	25	4.6	0.03	1.44
Benzene 0.0308 25 7.6 0.000 1.46 p -Xylene 0.0408 25 8.5 0.02 1.43 0.0408 55 6.2 0.02 1.41 Mesitylene 0.0479 25 10.4 0.12 1.43 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 I,1,2,2-TetrachloroethaneCyclohexane 0.0248 25 5.6 0.06 1.59 0.0248 25 5.6 0.06 1.59 0.0248 55 4.0 0.09 1.60 Benzene 0.0213 25 10.4 0.05 1.71 0.0266 25 13.4 0.08 1.74 0.0266 25 13.4 0.08 1.74 0.0266 55 8.0 0.12 1.71 Mesitylene 0.0300 25 19.7 0.12 1.65 0.0300 55 11.7 0.08 1.63 p -Dioxane 0.0164 25 18.6 0.00 1.88 PentachloroethaneCyclohexane 0.0489 25 6.6 0.00 1.03 Benzene 0.0425 25 7.7 0.06 1.15 p -Dioxane 0.0587 25 15.4 0.08 1.17 0.0587 55 9.5 0.08 1.13 Mesitylene 0.0674 25 2	Demonstra	0.0358	22	3.7	0.00	1.44
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Benzene	0.0308	25	7.6	0.00	1.40
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	n Vulana	0.0308)) 25	5.2	0.00	1.45
Mesitylene 0.0408 53 6.2 0.02 1.41 Mesitylene 0.0479 25 10.4 0.12 1.43 p -Dioxane 0.0257 25 13.7 0.04 1.53 $1,1,2,2$ -Tetrachloroethane $1,1,2,2$ -Tetrachloroethane $1,1,2,2$ -TetrachloroethaneCyclohexane 0.0248 25 5.6 0.06 1.59 0.0248 25 10.4 0.09 1.60 Benzene 0.0213 25 10.4 0.05 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0266 55 8.0 0.12 1.71 Mesitylene 0.0300 25 19.7 0.12 1.65 0.0300 25 19.7 0.12 1.65 p -Dioxane 0.0164 25 18.6 0.00 1.88 Pentachloroethane 0.0489 25 6.6 0.00 1.03 Benzene 0.0425 25 12.7 0.08 1.07 0.0425 55 7.7 0.06 1.15 p -Xylene 0.0587 25 15.4 0.08 1.17 0.0587 55 9.5 0.08 1.13 Mesitylene 0.0674 25 21.7 0.10 1.11 0.0674 25 16.7 0.09 1.09 p -Dioxane 0.0376 25 27.6 0.08 1.26	<i>p</i> -Aylene	0.0408	25	8.5	0.02	1.43
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Mecitulana	0.0408	25	10.4	0.02	1.41
$\begin{array}{c cccccc} p-Dioxane & 0.0277 & 25 & 13.7 & 0.03 & 1.43 \\ \hline p-Dioxane & 0.0257 & 25 & 13.7 & 0.04 & 1.53 \\ \hline 1,1,2,2-Tetrachloroethane \\ Cyclohexane & 0.0248 & 25 & 5.6 & 0.06 & 1.59 \\ \hline 0.0248 & 55 & 4.0 & 0.09 & 1.60 \\ Benzene & 0.0213 & 25 & 10.4 & 0.05 & 1.71 \\ \hline 0.0213 & 55 & 7.0 & 0.09 & 1.71 \\ p-Xylene & 0.0266 & 25 & 13.4 & 0.08 & 1.74 \\ \hline 0.0266 & 55 & 8.0 & 0.12 & 1.71 \\ Mesitylene & 0.0300 & 25 & 19.7 & 0.12 & 1.65 \\ \hline 0.0300 & 55 & 11.7 & 0.08 & 1.63 \\ p-Dioxane & 0.0164 & 25 & 18.6 & 0.00 & 1.88 \\ \hline Pentachloroethane \\ Cyclohexane & 0.0489 & 25 & 6.6 & 0.00 & 1.07 \\ \hline 0.0489 & 55 & 4.9 & 0.00 & 1.03 \\ Benzene & 0.0425 & 25 & 12.7 & 0.08 & 1.07 \\ \hline 0.0425 & 55 & 7.7 & 0.06 & 1.15 \\ p-Xylene & 0.0587 & 55 & 9.5 & 0.08 & 1.13 \\ Mesitylene & 0.0674 & 25 & 21.7 & 0.10 & 1.11 \\ \hline 0.0674 & 55 & 16.7 & 0.09 & 1.09 \\ p-Dioxane & 0.0376 & 25 & 27.6 & 0.08 & 1.26 \\ \end{array}$	wiesitylene	0.0479	25	10.4	0.12	1.43
P Elonate $1,1,2,2$ -Tetrachloroethane $1,1,2,2$ -TetrachloroethaneCyclohexane 0.0248 25 5.6 0.06 1.59 0.0248 55 4.0 0.09 1.60 Benzene 0.0213 25 10.4 0.05 1.71 p -Xylene 0.0266 25 13.4 0.08 1.74 0.0266 55 8.0 0.12 1.71 Mesitylene 0.0300 25 19.7 0.12 1.65 p -Dioxane 0.0164 25 18.6 0.00 1.88 PentachloroethaneCyclohexane 0.0489 25 6.6 0.00 1.07 0.0425 25 12.7 0.08 1.07 0.0425 25 7.7 0.06 1.17 p -Xylene 0.0587 25 15.4 0.08 1.17 0.0587 55 9.5 0.08 1.13 Mesitylene 0.0674 25 21.7 0.10 1.11 0.0674 55 16.7 0.09 1.09 p -Dioxane 0.0376 25 27.6 0.08 1.26	<i>p</i> -Dioxane	0.0257	25	13 7	0.03	1.43
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	p-Dioxane	0.0164	25	18.6	0.00	1.88
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Cvclohexane	0.0489	25	6.6	0.00	1.07
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Benzene	0.0425	25	12.7	0.08	1.07
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0.0425	55	7.7	0.06	1.15
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	<i>p</i> -Xylene	0.0587	25	15.4	0.08	1.17
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p-Dioxane 0.0674 55 16.7 0.09 1.09 0.0376 25 27.6 0.08 1.26	Mesitylene	0.0674	25	21.7	0.10	1.11
<i>p</i> -Dioxane 0.0376 25 27.6 0.08 1.26	-	0.0674	55	16.7	0.09	1.09
	p-Dioxane	0.0376	25	27.6	0.08	1.26



Figure 1. (A) Plot of the most probable relaxation time of the solute at 25° (1,2-dichloroethane at 20°) against the ionization potential of the solvent (cyclohexane, 9.88 eV; benzene, 9.25 eV; p-xylene, 8.86 eV; mesitylene, 8.39 eV: •, pentachloroethane; •, 1,1,2,2-tetrachloroethane; \triangle , 1,1,1,2-tetrachloroethane; \triangle , 1,1,2-tetrachloroethane; \bigcirc , 1,2-dichloroethane; \bigcirc , 1,2-dichloroethane; (B) Similar to Figure 1A, but at 55°.

Discussion

Small distribution parameters are obtained for almost all of the systems which have been examined (Table I), and the possibility of more than one contributing relaxation

	Benzene		<i>p</i> -Xylene		Mesitylene		p-Dioxane	
Ethane solute	25°	55° `	25°	55°`	25°	55° \	25°	
1,1-Dichloro-	280		310		340		470	
1,2-Dichloro- ^a	300ª	380 ^b	490ª	470	590ª	600	710ª	
1,1,1-Trichloro-	140	170	170	150	300	270	410	
1,1,2-Trichloro-	320	320	430	320	500	370	500	
1,1,1,2-Tetrachloro-	310	230	370	330	490	450	660	
1,1,2,2-Tetrachloro-	370	370	520	450	750	710	720	
Pentachloro-	390	300	500	430	710	800	850	

^a Refer to results at 20°. ^b Obtained from τ_0 in cyclohexane and benzene at 55 and 50°, respectively.

Table III. Effect of Solvent upon the Relaxation Time and Apparent Dipole Moment for Some Chloroethanes

	$\tau_{0B}/\tau_{0cycs}, 25^{\circ}$				Δμ/μ _{cyc} , 25°			
Ethane solute	Benzene	p-Xyler	ne Mesityler	ne p-Dioxane	Benzene	p-Xylene	Mesitylene	p-Dioxane
1,1-Dichloro-	1.60	1.68	1.76	2.20	-0.04	-0.03	-0.02	+0.02
1.2-Dichloro- ^a	1.67ª	2.29	^a 2.76 ^a	3.294	$+0.25^{a}$	$+0.08^{a}$	$+0.02^{a}$	$+0.25^{a}$
1,1,1-Trichloro-	1.27	1.36	1.64	2.00	-0.01	-0.04	-0.04	+0.02
1,1,2-Trichloro-	1.72	2.05	2.32	2.32	+0.11	+0.06	+0.01	+0.19
1,1,1,2-Tetrachloro-	1.68	1.86	2.27	3.00	+0.01	-0.01	-0.01	+0.06
1,1,2,2-Tetrachloro-	1.86	2.39	3.52	3.32	+0.08	+0.09	+0.04	+0.18
Pentachloro-	1.92	2.33	3.29	4.18	0.00	+0.09	+0.04	+0.18
- 			·····					
			$\tau_{OB}/\tau_{Oc,c}$, 55°			— Δμ/μ _{eye} , 55	•	
Solute	Be	nzene	<i>p</i> -Xylene	Mesitylene	Benzene	<i>p</i> -Xylene	Mesityle	ene
1,2-Dichloro-	1	l.81 ^b	2.06	2.50	+0.21	+0.07	+0.0	3
1,1,1-Trichloro-	1	1.30	1.25	1.50	-0.03	-0.01	-0.0	4
1,1,2-Trichloro-	1	l . 50	1.62	1.75	+0.07	+0.06	+0.0	4
1,1,1,2-Tetrachloro	- 1	l.41	1.66	1.98	+0.01	-0.02	-0.0	1
1,1,2,2-Tetrachloro	- 1	1.75	2.00	2.93	+0.07	+0.07	+0.0	2
Pentachloro-	1	l. 5 7	1.94	3.41	+0.12	+0.10	+0.0	6

^a Refer to results at 20°. ^b Obtained from τ_0 in cyclohexane and benzene at 55 and 50°, respectively.

process in such cases must be considered. A contribution from an intramolecular process may be discarded for 1,1,1-trichloroethane, since there is no component moment perpendicular to the C-C axis, and for 1,1,1,2-tetraand 1,1,2,2-tetrachloroethanes and pentachloroethane in view of their large potential barriers to internal rotation.^{6,17} The fact that a plot of τ_0 (in cyclohexane) against volume for all the chloroethanes is approximately linear¹⁸ is evidence against any appreciable contribution from an intramolecular process for 1,1-dichloro-, 1,2dichloro-, and 1,1,2-trichloroethanes or from a discrete process originating from solute-solute interaction, which would hardly be a constant throughout the series. Furthermore, the distribution parameters show no trend with increased solute-solvent interaction (Table I) and are probably due to variations in local environment among the solute molecules, an effect which seems not uncommon for small polar molecules in nonpolar solvents.¹⁹

For the systems which have also been studied by Chitoku and Higasi⁵ and Crossley and Walker⁶ the agreement for the dipole moments is reasonable in view of the short relaxation times and the enhanced errors in the extrapolated ε_{∞} values. In general, we have used more dilute solutions than those of Crossley and Walker, and our relaxation times are somewhat shorter, the effect being most noticeable for the strong interactors 1,1,2,2tetrachloroethane and pentachloroethane, indicating that solute-solute interaction is not negligible.

For all the chloroethanes, with the exception of 1,1,2,2tetrachloroethane, for which the relaxation time in mesitylene is longer than in p-dioxane, the relaxation times lengthen in the solvent order: cyclohexane < benzene < p-xylene < mesitylene < p-dioxane. The viscosities of the aromatic solvents (~ 0.6 cP) are less than those of cyclohexane, 0.9 cP, and p-dioxane, 1.2 cP at 25°. Thus, viscosity effects alone do not account for the relaxation behavior and, indeed, for such small nearly spherical molecules, especially 1,1,1-trichloroethane, the relaxation times might be almost independent of the macroscopic viscosity.²⁰ For the hydrocarbon solvents the relaxation time increases are comparable with their relative basicities,^{21,22} indicating some type of donor-acceptor interaction where the aromatic solvents may act as proton acceptors. The basicities of the solvents should, to some extent, be reflected in their ionization potentials,²³ and these are plotted against the relaxation times for each ethane in Figure 1A and 1B. The linearity of these plots is comforting in that they confirm solute-solvent interactions as the major contributing factor in lengthening the relaxation times. However, no inference as to the specific nature of the interaction can be drawn solely on the basis of such a relationship. The ionization potential for p-

^{2181 (1968).}

⁽²⁰⁾ A. J. Curtis, P. L. McGeer, G. B. Rathmann, and C. P. Smyth, J. Am. Chem. Soc., 74, 644 (1952).
(21) M. Tamres, *ibid.*, 74, 3375 (1952).
(22) H. C. Brown and J. D. Brady, *ibid.*, 74, 3570 (1952).
(23) V. J. Vendeneyev, L. V. Gurich, V. N. Kondratiyev, V. A. Medvedev, and Ye. L. Frankevich, "Bond Energies, Ionization Potential and Electron Affective". Pedvend Arrold Ltd. L codor, 1966. tials, and Electron Affinities," Edward Arnold Ltd., London, 1966.



Figure 2. Plot of $\Delta \mu/\mu_{eyc}$ against τ_{0B}/τ_{0cyc} for chloroethanes in benzene solution at (A) 25° (1,2-dichloroethane 20°) and (B) 55°. The solutes are identified as in Figure 1A.



Figure 3. Plot of $\Delta \mu/\mu_{cyc}$ against τ_{0B}/τ_{0cyc} for chloroethanes in *p*-xylene solution at (A) 25° (1,2-dichloroethane 20°) and (B) 55°. The solutes are identified as in Figure 1A.

dioxane is 9.52 eV, and the relaxation times in p-dioxane do not conform with the hydrocarbon solvent data, although the situation would be much improved if a viscosity correction were included. However, interaction with *p*-dioxane will involve the oxygen lone-pair electrons, not delocalized π electrons, and the systems are not completely analogous. For each ethane the degree of interaction with a solvent may be represented by τ_{0B}/τ_{0cvc} , where τ_{0B} and τ_{0cyc} are the most probable relaxation times in the potentially basic solvent and in the reference solvent cyclohexane, respectively. These ratios may be used in eq 2 to calculate the free energy of activation differences $\Delta \Delta G_0^{\dagger}$ for molecular relaxation. The values thus obtained are of the order expected for these systems and compare well with similar values obtained by nmr.²⁴ (24) I. D. Kuntz, results to be published.

The relative interactions for the chloroethanes in a given solvent are compared with the dipole moment changes in Table III and Figures 2-5, in which $\Delta \mu = \mu_B - \mu_{eye}$, where μ_B and μ_{eye} refer to solvents in the same manner as τ_{0B} and τ_{0eye} . The errors involved in these plots are necessarily large, but, apart from the *p*-dioxane results, there seems to be a clear increase in $\Delta \mu / \mu_{eye}$ for each solvent system with increasing interaction, and this solvent effect decreases in the order: benzene > *p*-xylene > mesitylene. It has been stated,³ and confirmed by nmr²⁴ work on chloroethanes, that a methyl group in any molecule cannot form hydrogen bonds. Thus, the fact that the relaxation time for 1,1,1-trichloroethane increases in the solvent order cyclohexane < benzene < *p*-xylene < mesitylene < *p*-dioxane suggests that, though hydrogen bonding may be important in some of the other systems,



Figure 4. Plot of $\Delta \mu/\mu_{eyc}$ against τ_{0B}/τ_{0cyc} for chloroethanes in mesitylene solution at (A) 25° (1,2-dichloroethane 20°) and (B) 55°. The solutes are identified as in Figure 1A.



Figure 5. Plot of $\Delta \mu/\mu_{cyc}$ against τ_{0B}/τ_{0cyc} for chloroethanes in *p*-dioxane solution at (A) 25° (1,2-dichloroethane 20°) and (B) 55°. The solutes are identified as in Figure 1A.

it is not the only contributing factor. Dipole-induceddipole interaction is a strong possibility in such cases, and the effect may be compared with the behavior of trichlorofluoromethane, a molecule incapable of forming hydrogen bonds, which has a larger reduced relaxation time⁴ in *p*dioxane (5.7 psec) than in carbon tetrachloride (3.3 psec) at 20°. There is no clear relationship between the relative interaction strengths and the apparent dipole moments of

the ethanes, indicating that hydrogen bonding is more important than dipolar forces in many cases. The relative interactions for the solutes are, with the exception of 1,2-dichloroethane, as would be expected from the protonic nature of the hydrogen atoms within the molecules and show an order similar to that of the nmr chemical shifts for these solutes in a 10% solution of dimethyl sulfoxide in cyclohexane.²⁵ Proton magnetic resonance studies^{24,25} indicate that 1,2-dichloroethane interacts with bases only to a slightly greater extent than 1,1,1-trichloroethane, and the results for the former (Tables II and III and Figures 2-5) are indeed surprising. Although very rough curves might be drawn in Figures 2-5, the complicating factors involved make it seem wiser to let the points alone indicate the general trend. Schneider⁷ proposed the introduction of a volume term to account for the mean distance of approach between the interacting molecules. Crossley and Walker⁶ found that such corrections yield more reasonable $\tau_{0B}V/\tau_{0cyc}$ values for 1,2-dichloroethane, where V is the volume of the molecule, but they also indicate 1,1-dichloroethane to be a weaker interactor than 1,1,1-trichloroethane.

The relatively large $\Delta \mu/\mu_{eye}$ values for 1,2-dichloroethane have been interpreted in terms of an increased proportion of the polar *gauche* form relative to the nonpolar *trans* form.⁵ This is often accounted for by the effect of increased dielectric constant on the electrostatic stabilization energy, causing the energy of the polar *gauche* form to decrease, relative to that of the nonpolar *trans* form. However, the dielectric constants of mesitylene and *p*-xylene are of the same order as that of benzene, but the dipole moments in the former solvents are less than in benzene. Furthermore, the dielectric constant of pure

(25) A. L. McClellan and S. W. Nicksic, J. Phys. Chem., 69, 446 (1965).

liquid 1,2-dichloroethane²⁶ at 25° is 10.16 and the dipole moment (1.88 D.) is not considerably different from the value in benzene solution. From Table I it is apparent that the dipole moment of this solute decreases in the same manner as those of 1,1,2,2-tetrachloroethane and 1,1,2trichloroethane in the solvent order *p*-dioxane > benzene > p-xylene > mesitylene > cyclohexane. For 1,1,2,2tetrachloroethane the potential barrier to internal rotation is large,¹⁷ and the solvent effect would seem to be due to

(26) F. Buckley and A. A. Maryott, "Tables of Dielectric Dispersion Data for Pure Liquids and Dilute Solutions," National Bureau of Standards, Circular 589, Government Printing Office, Washington, D. C., 1958.

molecular interaction rather than any increased freedom for intramolecular rotation. From Figures 2-4, although the degree of interaction does appear to be anomalously large, the dipole moment changes for 1,2-dichloroethane are reasonable and suggest that they are not solely due to intramolecular effects.

In a specific solvent increasing molecular interaction appears to be accompanied by increased dipole moment changes for the chloroethane series. However, this effect decreases in the solvent order benzene > p-xylene > mesitylene, suggesting that the induced dipole moments decrease with increasing basicity or mean polarizability for these systems.

Some Thermochemical Properties of Methyl Vinyl Ether, α-Chloroethyl Methyl Ether, and Iodomethyl Methyl Ether. Evidence for Nonbonded Electrostatic Interactions¹

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Abstract: The entropies of methyl vinyl ether (MVE, $S^{\circ}_{298} = 73.5$ gibbs/mole) and α -chloroethyl methyl ether (CME, $S^{\circ}_{298} = 82.4 \pm 2.1$ gibbs/mole) have been calculated, respectively, by statistical mechanical methods, and from the measured equilibrium constant, K_{α} , CH₃OCHClCH₃ \Rightarrow HCl + CH₃OCH=CH₂ (α). In the latter measurement, HCl pressures were varied from 104.5 to 227.8 torr, and MVE from 28.57 to 213 torr. Log (K_{α}/atm) = $[(34.0 \pm 1.5)/4.576] - [(17.5 \pm 0.7)/\theta]$, where $\theta = 2.303RT$ in kilocalories/mole, and errors quoted are 95% confidence limits. Smoothing these values to $\Delta H = 17.0 \text{ kcal/mole}$ by comparison with the similar equilibrium for ethyl vinyl ether leads to $\Delta H_{f^{\circ}298}(\text{CME}) = -65.2 \pm 1.2 \text{ kcal/mole}$. The heat of formation of iodomethyl methyl ether ($\Delta H_{\rm f}^{\circ}_{298}(\rm{IME}) = -29.3$ kcal/mole) was calculated from the equilibrium constant, $K_{\rm eq}$, at 566°K for the system $CH_3OCH_3 + I_2 \rightleftharpoons HI + ICH_2OCH_3$ (IME) and an assigned value for the entropy of the iodomethyl ether. I_2 pressures were varied from 3.76 to 18.85 torr and dimethyl ether pressures from 39.62 to 592 torr. The temperature range was 515–631.6°K. S°_{298} (CME) was abnormally low by 1.9 gibbs/mole on comparison with isoelectronic sec-butyl chloride, and ΔH_{f}° (CME) was abnormally stable by about 6.1 kcal/mole. ΔH_{f}° (IME) showed a similar enhanced stability of about 3 kcal/mole. Both of these values are shown to be consistent with an electrostatic interaction of the halogens with the terminal methyl group arising from the alternate polarity of bond dipoles.

ata on the entropies and heat capacities of ethers are particularly scarce,² only those of dimethyl ether having been calculated³ by the method of Pitzer and Gwinn⁴ from a spectroscopic frequency assignment.

Entropies of other ethers have been estimated by group additivity methods² or else by an "isoelectronic replacement rule." The success of this rule depends on the observation that, at 298°K, replacement of the oxygen atom in an oxygen-containing compound by an isoelectronic group, here the methylene group, does not significantly alter the entropy, provided due account is

taken of any symmetry changes involved and the very small contribution of the H atoms. Table I shows that the rule is generally accurate within ± 1 gibbs/mole. The agreement is expectedly poor for the acids (and presumably esters), which have high OH (or OR) rotation barriers. The poor result for H_2O_2 is due to the large difference in moments of inertia between H_2O_2 and C_2H_6 .

The external moment of inertia about the C-C axis in C_2H_6 is three times larger than that about the O-O axis in H_2O_2 . This is also approximately the case for the internal rotation, and correction for both of these effects amounts to about 2.5 gibbs/mole. A crude a priori estimate of the effect of losing two H atoms in a molecule can be made by assigning one C-H stretch at 3000 cm⁻¹ and two H-C-C deformations at about 1000 cm⁻¹. At 300°K these amount to about 03 gibbs/mole per H atom, or 0.6 gibbs/mole for two H atoms, in good agreement with most of the ΔS values shown.

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