

Characterization of Polymer–Solvent Interactions and Their Temperature Dependence Using Inverse Gas Chromatography

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Inverse gas chromatography has been used to measure specific retention volumes and to derive a comprehensive set of interaction parameters for 9 polymers and 43 solvents at 6 temperatures from 60 to 110 °C. The specific retention volume, the Flory–Huggins interaction parameter χ_{12} , and the excess cohesive energy parameter B_{12} are presented for each polymer–solvent system as a function of temperature.

Introduction

Inverse gas chromatography (IGC), introduced about 20 years ago, is a rapid and reliable method for measuring polymer–solvent interactions (1–3). In a previous paper (4), we reported interaction parameters at 100 °C for 19 polymers and 43 solvents. We developed a multicomponent solubility parameter theory for polymer–solvent interactions (5) based on these data. As a continuation of our systematic investigations, in this paper we present interaction parameters gathered on 9 polymers with 43 solvents at six different temperatures. Analysis of these data will be presented in a separate paper.

During our IGC experiments, we have found that improvements in both the collection of experimental values and the data analysis (4, 6–9) are necessary to obtain more accurate thermodynamic values. The major sources of errors in common IGC experiments include (1) inaccurate determination of polymer mass on the IGC column by conventional solvent-extraction method, (2) poor constancy of the carrier-gas flow rate caused by room temperature fluctuations, and (3) improper analysis of the experimental results including neglect of the retention of the marker and of the retention of probes (the injected solvents) by the inert support. After elimination of these experimental errors and with proper data treatment, we estimate the accuracy of the specific retention volumes to be within 1%.

Theory

The change of the Gibbs free energy upon mixing, according to the Flory–Huggins theory, can be expressed as (10)

$$\Delta_{\text{mix}}G = RT[n_1 \ln \Phi_1 + n_2 \ln \Phi_2 + n_1 \Phi_2 \chi_{12}] \quad (1)$$

where Φ_1 and Φ_2 are the volume fractions of solvent and polymer, respectively, n_1 and n_2 are the numbers of moles of solvent and polymer, respectively, RT has its usual meaning, and χ_{12} is the Flory–Huggins interaction parameter.

Phenomenologically, the above equation has been considered as the definition of χ_{12} . All properties of a mixture can be expressed in terms of the variations of χ_{12} with composition, temperature, and pressure (11, 12). At the vanishing concentration of the probe, χ_{12} can be obtained

from the IGC experiment as

$$\chi_{12} = \ln(RTv_2/V_1P_1^\circ V_g) - 1 + V_1/M_2v_2 - (B_{11} - V_1)P_1^\circ/RT \quad (2)$$

where V_g is the specific retention volume of the probe, which is obtained directly from experiment, V_1 and v_2 are the solvent molar volume and polymer specific volume, respectively, P_1° is the saturated vapor pressure of the probe, and B_{11} is the second virial coefficient of the probe in the vapor phase. The parameter of negative excess cohesive energy B_{12} is defined as

$$B_{12} = RT\chi_{12}/V_1 \quad (3)$$

The specific retention volume is determined as

$$V_g = j(t_p - t_m)F/w \quad (4)$$

where w is the mass of the polymer on the column and F is the flow rate of the carrier gas at the column temperature at the column outlet. t_p and t_m are the retention times of the probe and the marker, respectively. j is a correction factor to account for the compressibility of the carrier gas and is given by

$$j = (3/2)[(P_i/P_o)^2 - 1]/[(P_i/P_o)^3 - 1] \quad (5)$$

where P_i and P_o are the column inlet pressure and outlet pressure, respectively.

In many IGC experiments, column temperatures above 100 °C and often up to 200 °C are used. The saturated vapor pressure of some probes under these circumstances is very high; the nonideal gas virial term cannot be omitted and should be treated with care. Equation 2 becomes meaningless when the column temperature exceeds the critical temperature of the probe.

Experimental Section

Materials. Polyepichlorohydrin was purchased from Scientific Polymer Products Inc. and Goodrich Inc.; poly(ethylene) was a gift from Dr. Fetters, Exxon Corp. All other polymers were purchased from Scientific Polymer Products Inc. Specific volumes of the polymers were either taken directly from the literature or calculated from the group contribution method. Polymer names, codes, and specific volumes are listed in Table 1.

All the probes were obtained from reputable suppliers. Only cyclopentane was of insufficient purity. It was distilled several times before use. Vapor pressures of the probes were obtained from their Antoine vapor pressure

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Table 1. Listing of Polymers, Their Codes, and Physical Constants^a

polymer	code	$T_g/$ °C	$\rho/$ (g/cm ³)	$d\rho/dT$ $\times 10^4$
poly(ethylethylene)	PEE	-4	0.872	6.69
polypropylene	PP1	-26	0.865	5.56
poly(dimethylsiloxane)	PDMS	-127	0.970	8.79 (22)
polycaprolactone	PCL	-60	1.095	8.64 (23)
polyepichlorohydrin	PECH	-22	1.360	10.4
poly(2-hydroxyethyl acrylate)	PHEA	-15	1.310	8.20
poly(methyl acrylate)	PMA	10	1.220	7.60 (24)
poly(ethyl acrylate)	PEA	-24	1.12	6.40
poly(<i>n</i> -butyl methacrylate)	PBMA	20	1.055	6.60 (25)

^a All ρ and $d\rho/dT$ were calculated from ref 14, unless indicated otherwise.

Table 2. Listing of Probes and Their Critical Temperatures, Critical Volumes, and Critical Pressures

probe	code	T_c/K	$V_c/(\text{cm}^3/\text{mol})$	P_c/MPa
propane	NC3	370.0	197.5	4.261
butane	NC4	425.2	255.0	3.800
pentane	NC5	469.7	304.0	3.370
hexane	NC6	507.5	370.0	3.010
heptane	NC7	540.2	426.0	2.736
octane	NC8	568.8	492.0	2.488
nonane	NC9	594.6	548.0	2.288
decane	C10	617.7	603.0	2.120
undecane	C11	638.8	660.0	1.966
cyclopentane	CC5	511.9	259.8	4.517
cyclohexane	CC6	553.6	309.6	4.075
cycloheptane	CC7	604.4	353.0	3.860
cyclooctane	CC8	647.2	410.0	3.557
cyclohexene	CHX	560.5	292.0	
cyclohexadiene	CHD	561.5	276.4	
benzene	BNZ	562.2	260.3	4.898
toluene	TOL	594.0	320.0	4.236
ethylbenzene	EBZ	617.2	374.5	3.609
methyl chloride	CL1	416.2	139.0	6.679
methylene chloride	CL2	510.2	185.8	6.079
chloroform	CL3	536.4	240.7	5.472
carbon tetrachloride	CL4	556.4	275.9	4.560
butyl chloride	BCL	542.0	312.0	3.680
pentyl chloride	PCL	572.3	355.5	
chlorohexane	CLH	599.5	403.6	
chlorooctane	CLO	644.6	514.0	
1,1-dichloroethane	D11	523.0	240.0	5.070
1,2-dichloroethane	D12	566.0	225.0	5.370
methylchloroform	MCH	545.0	272.5	
trichloroethylene	TCE	572.0	256.0	5.050
chlorobenzene	CLB	632.4	308.1	4.520
acetone	ACT	508.1	209.0	4.700
methyl ethyl ketone	MEK	536.8	267.1	4.207
tetrahydrofuran	THF	540.2	224.0	4.770
dioxane	DOX	587.0	238.0	5.210
methyl acetate	MAC	506.8	228.0	4.690
ethyl acetate	EAC	523.2	286.0	3.830
propyl acetate	PAC	549.4	345.0	3.335
<i>n</i> -butyl acetate	NBA	579.0	400.0	3.140

coefficients at the proper temperature ranges. These coefficients together with other necessary constants were extracted from the Dreisbach compilation and other sources (14–18). Table 2 lists the probes and their codes, together with their critical temperatures, critical volumes, and critical pressures, which were used for the calculations of the gas virial coefficients.

Column Preparations. IGC columns were prepared from 0.64-cm-o.d. copper tubing 150 cm long, which was cleaned with methanol and left overnight in an oven at 110 °C. The support used was 60–80-mesh Chromosorb-W (acid washed and treated with dichlorodimethylsilane). The soaking method described previously was used for coating by the polymers. Polymer loadings were about 7% by mass.

Data Acquisition. The IGC experiments were performed on a modified Varian Aerograph 2100-40 gas

chromatograph equipped with a flame ionization detector (FID). Methane was used as a marker. The elution signal from the FID output was monitored by a Hewlett-Packard 3478A digital voltmeter and was processed in real time by a personal computer. Nitrogen was used as the carrier gas, and the flow rate was between 15 and 18 mL/min. The precision in the flow-rate measurement was ± 0.02 mL/min. Injected volumes were in the range of 0.02–0.04 μL and the retention volumes (after correction for the retention by the support; see below) were essentially independent of the injection sizes in a broad range. The temperature of the column was controlled within ± 0.1 °C.

During the data analysis, we have performed all the necessary corrections in the same way as we described previously (4, 5) except the correction for support retentions.

Retention by the Support. In our previous IGC experiments, we have found that the retention of the support is non-negligible in most cases and must be accounted for. The typical retention of the support for nonpolar probes accounts for 1–5% of the net retention volumes of the probe. For polar probes, it varied from 1% up to 20% depending on the amount of probe injected. Correction of the retention results for support adsorption can be performed by direct subtraction of the support retention from the apparent specific retention of the column, V_g^a , such that

$$V_g = V_g^a - V_n^s/w \quad (6)$$

where V_n^s is the retention of the probe on the support as obtained from an independent experiment on the uncoated support.

The support retentions depend on both temperature and the amount of probe injected. The concentration dependence of the support retentions varied with the chemical nature of the probe, being most pronounced for the strongly polar probes and negligible for alkanes and other hydrocarbons. Within the region of sample sizes practical to IGC experiments, all the concentration dependences of the probes were found to obey the relation

$$\ln V_n^s = a_1 + b_1 \ln A_p \quad (7)$$

where A_p , the peak area, is a measure of the probe sample size. a_1 and b_1 are temperature-dependent constants. In this study, we have found that the temperature dependence of support retentions obeys the Arrhenius relation

$$\ln V_n^s = a_2 + b_2/T \quad (8)$$

Combining eqs 7 and 8, we obtain

$$\ln V_n^s = a + b/T + c \ln A_p \quad (9)$$

Here, a_2 , b_2 , a , b , and c are probe-specific constants applicable for a given support and a given way of expressing the peak areas.

We have performed IGC experiments for each probe on the uncoated support at several temperatures. At each column temperature, we have injected different amounts of the probes. Thus, for each probe, we obtained a set of constants a , b , and c . The retention of the support for a given probe is then calculated from eq 9. At high temperatures, the retentions of lower carbon number hydrocarbons (propane, butane, etc.) by the support cannot be determined with good accuracy, because of extremely small retention volumes (< 0.1 mL/g) of these probes. Nevertheless, we have found that for the same homologous group of compounds at low temperature, the retentions by the support are related to the carbon number with excellent

Table 3. Specific Retention Volume V_g of Various Probes on a PEE Column

$V_g/(\text{cm}^3 \text{g}^{-1})$						$V_g/(\text{cm}^3 \text{g}^{-1})$							
$t/^\circ\text{C} =$ 60.0	$t/^\circ\text{C} =$ 70.0	$t/^\circ\text{C} =$ 80.0	$t/^\circ\text{C} =$ 90.0	$t/^\circ\text{C} =$ 100.0	$t/^\circ\text{C} =$ 110.0	$t/^\circ\text{C} =$ 60.0	$t/^\circ\text{C} =$ 70.0	$t/^\circ\text{C} =$ 80.0	$t/^\circ\text{C} =$ 90.0	$t/^\circ\text{C} =$ 100.0	$t/^\circ\text{C} =$ 110.0		
NC3	4.90	4.06	3.71	3.50		BCL	117.15	88.15	67.89	53.10	42.06	34.23	
NC4	13.47	10.80	9.53	8.19		PCL	294.14	211.80	155.80	116.63	88.72	69.63	
NC5	34.52	26.90	21.98	17.73	14.85	12.34	CLH	722.32	495.98	349.11	250.43	182.93	138.55
NC6	86.87	65.17	50.39	39.59	31.34	25.25	CLO	4214.19	2644.18	1723.32	1138.36	761.30	535.33
NC7	214.54	153.73	114.56	85.77	65.18	50.60	D11	56.27	44.22	35.32	28.72	23.47	19.69
NC8	522.71	357.23	255.39	182.84	133.68	100.23	D12	102.50	78.50	61.23	48.68	38.70	31.98
NC9	1263.64	825.41	565.08	386.77	272.42	196.55	MCH	116.98	89.63	68.45	54.93	43.55	35.83
C10	2991.01	1906.43	1241.73	815.31	550.53	384.21	TCE	207.44	153.32	114.18	88.97	68.91	55.28
C11		4360.78	2697.40	1755.65	1123.99	752.73	CLB	696.61	489.22	348.60	258.08	191.65	147.93
CC5	71.88	55.69	44.62	35.27	28.20	23.70	ACT	15.96	13.33	11.70	10.05	8.40	7.60
CC6	178.66	133.29	102.71	78.74	61.52	49.24	MEK	48.38	37.94	30.02	24.60	19.84	16.89
CC7	602.92	424.55	306.93	226.73	168.80	130.52	THF	89.66	68.64	53.26	42.68	33.86	28.19
CC8	1780.02	1189.13	810.83	577.37	412.66	307.44	DOX	152.39	112.39	85.60	67.29	51.83	42.77
CHX	193.82	143.93	109.24	84.18	65.75	52.79	MAC	25.21	20.15	16.49	13.60	11.11	9.70
CHD	163.21	122.06	93.63		57.11	46.42	EAC	54.88	41.89	32.83	26.37	20.82	17.51
BNZ	140.70	106.28	81.97	64.31	50.87	41.47	PAC	137.34	100.48	74.94	57.81	44.24	35.67
TOL	359.94	258.93	191.82	143.22	108.80	85.62	NBA	341.47	238.14	169.61	125.47	92.56	72.06
EBZ	804.68	556.78	395.33	284.79	209.45	159.25	EOH	9.27	7.45	7.58	6.31	4.65	4.93
CL1	6.84	5.85	5.73	4.74	4.56	3.84	POH	30.40	23.75	19.99	16.28	13.08	11.64
CL2	34.24	27.43	22.90	18.62	15.70	13.55	BOH	82.11	61.89	48.22	38.12	29.65	25.26
CL3	84.81	65.57	52.14	41.36	33.34	27.80	AOH	201.14	152.17	112.39	85.47	64.61	52.02
CL4	155.48	117.57	90.87	70.51	55.66	45.33							

Table 4. Specific Retention Volume V_g of Various Probes on a PP1 Column

$V_g/(\text{cm}^3 \text{g}^{-1})$					$V_g/(\text{cm}^3 \text{g}^{-1})$							
$t/^\circ\text{C} =$ 70.0	$t/^\circ\text{C} =$ 80.0	$t/^\circ\text{C} =$ 90.0	$t/^\circ\text{C} =$ 100.0	$t/^\circ\text{C} =$ 110.0	$t/^\circ\text{C} =$ 70.0	$t/^\circ\text{C} =$ 80.0	$t/^\circ\text{C} =$ 90.0	$t/^\circ\text{C} =$ 100.0	$t/^\circ\text{C} =$ 110.0			
NC3	3.95	3.62	2.65		BCL	84.52	62.31	50.38	41.62	32.69		
NC4	9.97	8.91	6.71		PCL	203.72	152.87	112.50	88.36			
NC5	25.66	20.61	16.78	11.36	CLH	486.20	332.68	244.46	184.30	142.21		
NC6	63.52	49.32	37.75	29.87	25.13	CLO	2661.39	1732.12	1136.18	778.78	571.05	
NC7	153.08	113.55	83.60	63.84		D11	41.28	33.59	26.61	22.91	18.43	
NC8	360.45	254.02	181.49	134.04	105.87	D12	74.92	59.20	46.07	38.46	30.35	
NC9	764.17	571.99	388.52	276.58	211.79	MCH	83.30	65.09	50.93	42.04	34.64	
C10	1956.05	1281.77	826.07	568.46	436.03	TCE	145.72	108.79	84.69	67.77	54.31	
C11	4524.80	2913.40	1750.84	1158.50	828.20	CLB	470.97	328.04	246.32	189.82	151.30	
CC5	52.90	41.79	32.90	26.48	22.12	ACT	11.63	11.64	9.13	8.71	7.55	
CC6	127.45	96.81		58.80	47.87	MEK	36.35	29.02	23.44	20.26	16.18	
CC7	408.05	295.72	214.92	162.87	130.33	THF	64.50	50.94	40.34	33.86	26.70	
CC8	1121.03	764.13	552.59	402.61	310.24	DOX	106.98	82.82	63.83	52.70	41.40	
CHX	136.82	103.78	79.30	63.31	51.03	MAC	17.98	16.51	12.49	11.60	9.80	
CHD	115.63	88.41	68.08	55.16	44.46	EAC	40.10	31.97	24.81	21.34	16.29	
BNZ	101.55	77.20	60.31	48.94	40.10	PAC	97.64	73.75	55.60	45.05	37.11	
TOL	249.44	185.68	138.91	107.89	86.48	NBA	234.53	171.51	122.56	95.17	73.36	
EBZ	542.19	387.19		212.96	161.92	EOH	8.22	7.83	5.25	4.99	4.74	
CL1	6.02	5.23	4.64	4.44	3.80	POH	21.41	19.69	15.27	13.14	11.98	
CL2	25.17	21.88	17.70	15.25	11.06	BOH	58.71	45.60	36.52	29.55	24.46	
CL3	60.32	47.37	38.93	32.01	26.89	AOH	147.14	108.84	82.43	65.62	52.15	
CL4	105.72	82.97	64.67	52.78	43.21							

accuracy as

$$\ln V_n^s = d + eN \quad (10)$$

where N is the number of carbons in the molecule and d and e are constants. We can therefore obtain the support retentions of low molecular weight hydrocarbons by extrapolating V_n^s vs. carbon number according to eq 10. By controlling the injected volume, we have ascertained that the retention of the support was never greater than 5% of the net retention volume of the probe on coated column. In most cases, the retention of the support was within 2% of the corrected retention volume of the probe.

We have also ascertained that our values of V_g were not adversely affected by slow diffusion of probes through the polymer layer (19–21). We have demanded that the height of the equivalent theoretical plate (HETP) (which is the measure of diffusion of the probes on the column and varies from probe to probe) be the same for a given probe when measured on coated and uncoated columns. We have found that all our measurements satisfied this criterion except

for PHEA and PMA at low temperatures. Even for these measurements, the estimated errors in V_g , χ_{12} , and B_{12} were rather small. Nevertheless, we are excluding these values when analyzing the temperature dependence of the interaction parameters.

Results

The experimental values of the specific retention volume V_g are collected in Tables 3–11. All thermodynamic information about polymer–solvent interactions, their temperature dependence, equation-of-state effects, Henry's constants for each probe, etc., can be directly derived from the V_g values. We have listed the interaction parameters χ_{12} defined by eq 1 in Tables 12–20 and excess free energy of mixing B_{12} in Tables 21–29. We have excluded the χ_{12} and B_{12} values of propane and butane at 100 and 110 °C since the column temperatures are near or exceed the critical temperatures of the probes. We have also excluded the interaction parameters of propane, butane, pentane, and hexane on poly(2-hydroxyethyl acrylate), because of

Table 5. Specific Retention Volume V_g of Various Probes on a PDMS Column

	$V_g/(\text{cm}^3 \text{g}^{-1})$							$V_g/(\text{cm}^3 \text{g}^{-1})$					
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$
NC3	5.23	4.78	3.99	3.69			BCL	101.98	76.84	58.81	45.94	37.00	30.02
NC4	13.26	11.32	9.22	8.00			PCL	235.81	169.85	124.29	93.63	72.39	56.54
NC5	31.26	25.25	20.06	16.42	14.11	11.50	CLH	535.79	368.65	258.81	187.75	139.65	105.00
NC6	72.34	56.01	42.58	33.69	27.47	22.07	CLO	2749.03	1711.94	1104.82	741.01	510.53	357.71
NC7	165.62	122.63	89.47	68.01	53.16	41.68	D11	54.42	42.58	33.60	27.18	22.51	18.32
NC8	373.96	265.73	185.51	135.48	102.27	76.92	D12	93.88	71.60	54.99	43.34	35.23	28.15
NC9	840.68	570.16	383.09	268.96	195.24	141.99	MCH	100.92	76.83	58.99	46.40	37.64	30.12
C10	1983.94	1226.89	785.25	530.71	369.86	261.14	TCE	155.08	114.24	85.56	65.93	52.35	41.40
C11	4034.45	2490.33	1585.64	1041.79	702.96	477.92	CLB	481.37	340.71	242.42	178.86	133.96	100.93
CC5	55.67	44.35	34.72	27.61	23.20	18.69	ACT	24.40	19.97	16.62	14.00	12.10	9.85
CC6	123.11	94.60	71.52	55.50	44.99	35.73	MEK	61.94	47.40	37.69	29.57	24.15	19.43
CC7	353.89	256.65	187.86	138.28	106.28	82.08	THF	89.23	67.31	51.45	40.82	32.96	26.31
CC8	934.77	635.00	443.56	314.80	232.35	173.01	DOX	161.35	117.78	88.36	67.35	53.04	41.36
CHX	140.30	105.03	79.98	62.16	49.44	40.24	MAC	36.68	28.60	22.80	18.34	15.37	12.44
CHD	126.07	94.74	72.59	56.59	45.22	37.10	EAC	74.58	55.73	42.39	33.11	26.64	21.18
BNZ	114.62	86.72	66.40	51.97	41.93	33.16	PAC	170.59	121.54	88.64	66.90	51.44	40.10
TOL	265.63	192.15	140.29	106.02	82.24	62.84	NBA	387.13	263.21	184.63	133.78	99.07	74.91
EBZ	558.76	388.59	273.79	199.64	148.57	110.88	EOH	17.70	14.87	12.31	10.43	9.38	7.13
CL1	8.02	6.92	6.01	5.41	5.09	4.46	POH	47.27	36.33	27.61	22.61	18.79	14.83
CL2	36.70	29.37	23.52	19.22	16.34	13.05	BOH	115.16	84.08	61.40	47.65	37.54	29.37
CL3	75.25	58.09	44.72	35.72	29.29	23.21	AOH	272.27	188.12	133.78	98.32	74.01	56.54
CL4	119.54	90.54	68.57	54.08	43.47	34.24							

Table 6. Specific Retention Volume V_g of Various Probes on a PCL Column

	$V_g/(\text{cm}^3 \text{g}^{-1})$						$V_g/(\text{cm}^3 \text{g}^{-1})$					
	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC3	1.50	1.37	1.17			BCL	82.56	63.21	48.49	37.05	29.54	
NC4	3.81	3.11	2.95			PCL	179.21	131.75	97.14	71.91	55.67	
NC5	8.58	7.06	6.12	4.88	4.11	CLH	378.02	263.73	189.98	136.40	102.29	
NC6	18.77	14.90	12.21	9.77	8.10	CLO	1683.46	1065.08	718.99	482.01	338.59	
NC7	40.34	31.33	24.30	19.06	15.37	D11	81.11	61.12	47.40	36.16	29.00	
NC8	86.23	64.21	47.96	36.39	28.61	D12	222.07	161.73	120.60	89.28	68.94	
NC9	181.15	129.62	93.25	68.44	52.08	MCH	98.63	73.98	56.95	43.50	34.63	
C10	381.10	260.44	180.12	128.04	94.46	TCE	186.02	134.63	98.49	74.95	57.86	
C11	788.14	522.71	347.38	240.52	169.40	CLB	788.14	537.63	380.37	272.21	201.16	
CC5	22.12	17.77	14.78	12.03	9.90	ACT	47.73	37.27	29.08	23.27	18.87	
CC6	45.69	36.17	28.69	23.13	18.80	MEK	98.22	73.60	55.10	42.76	33.84	
CC7	140.22	105.72	80.46	62.50	48.60	THF	89.42	67.40	51.51	40.42	32.48	
CC8	375.18	271.91	197.52	146.76	110.48	DOX	296.05	210.31	151.72	112.96	86.50	
CHX	74.27	57.30	44.74	35.38	28.06	MAC	52.75	39.70	30.46	23.74	19.06	
CHD	97.06	74.14	56.84	44.55	35.26	EAC	85.67	62.62	46.92	35.92	28.17	
BNZ	142.13	105.80	80.53	61.71	48.25	PAC	172.06	121.58	88.27	65.78	50.16	
TOL	310.86	222.25	163.14	121.16	90.98	NBA	362.62	246.66	173.52	125.20	92.74	
EBZ	588.37	405.66	288.65	208.53	152.43	EOH	69.70	51.04	37.92	29.02	22.19	
CL1	9.02	7.69	6.73	5.50	4.76	POH	158.23	110.56	79.94	58.95	44.72	
CL2	79.23	60.41	46.35	35.54	28.46	BOH	354.54	237.99	166.59	118.71	87.48	
CL3	167.70	123.71	91.41	67.79	52.38	AOH	784.83	506.12	340.83	235.00	167.18	
CL4	94.88	72.50	55.13	42.25	33.37							

Table 7. Specific Retention Volume V_g of Various Probes on a PECH Column

	$V_g/(\text{cm}^3 \text{g}^{-1})$							$V_g/(\text{cm}^3 \text{g}^{-1})$					
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$
NC3	0.68	0.54	0.77	0.49			EBZ	504.92	349.23	244.93	175.07	129.41	96.85
NC4	1.86	1.73	1.59	1.41			CL1	6.30	5.46	5.13	4.39	3.90	3.40
NC5	4.00	3.54	3.27	2.70	2.47	2.06	CL2	50.08	38.35	30.09	23.53	18.90	15.58
NC6	9.95	8.14	6.79	5.62	4.71	4.18	CL3	84.52	63.64	48.11	36.87	29.09	23.42
NC7	21.70	17.10	13.73	10.93	9.10	7.67	CL4	58.86	45.56	35.39	27.92	22.47	18.51
NC8	45.58	34.55	26.51	20.64	16.47	13.50	BCL	64.50	48.40	37.12	29.05	23.18	18.80
NC9	94.82	69.32	51.03	38.63	29.79	23.48	PCL	139.00	99.84	74.11	55.78	43.27	34.19
C10	197.74	138.98	98.13	71.68	53.66	41.18	CLH	292.99	201.90	144.40	105.03	79.06	60.34
C11	409.73	275.82	188.36	132.47	96.25	71.42	CLO	1276.33	806.05	531.28	366.64	257.76	185.58
CC5	14.20	11.73	9.68	8.14	6.75	5.84	D11	55.87	41.85	32.63	25.37	20.56	16.86
CC6	30.59	24.65	19.93	16.15	13.29	11.35	D12	171.48	122.00	90.34	67.36	52.40	41.08
CC7	98.21	75.08	57.59	44.82	35.61	28.84	MCH	65.57	50.24	38.79	30.23	24.32	19.90
CC8	273.39	198.77	145.67	109.22	83.75	65.19	TCE	114.75	83.09	62.04	47.61	37.59	30.11
CHX	55.11	42.92	33.43	26.64	21.44	17.67	CLB	645.59	434.61	303.37	219.91	162.72	122.33
CHD	78.80	60.35	46.04	36.29	28.83	23.37	ACT	65.51	48.69	37.17	28.92	23.29	18.88
BNZ	124.59	93.02	70.02	53.39	41.74	33.27	MEK	133.18	95.32	70.19	52.84	41.14	32.58
TOL	274.59	196.18	141.95	104.50	79.17	60.87	THF	111.87	81.50	61.09	46.58	36.89	29.39

Table 7 (Continued)

	$V_g/(cm^3 g^{-1})$						$V_g/(cm^3 g^{-1})$						
	$t/^\circ C = 60.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	$t/^\circ C = 60.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	
DOX	396.77	268.79	189.36	136.34	102.11	76.75	EOH	44.28	32.87	24.62	18.87	14.16	11.96
MAC	59.60	43.82	32.87	25.29	20.20	16.05	POH	99.07	69.87	51.35	38.21	29.70	23.22
EAC	98.18	69.72	51.41	38.49	29.99	23.36	BOH	223.49	150.90		77.00	57.96	43.49
PAC	201.90	138.02	98.22	71.43	54.03	40.87	AOH	484.90	319.31		151.24	110.36	81.25
NBA	422.39	277.17	190.86	134.17	98.38	72.86							

Table 8. Specific Retention Volume V_g of Various Probes on a PHEA Column

	$V_g/(cm^3 g^{-1})$						$V_g/(cm^3 g^{-1})$						
	$t/^\circ C = 60.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	$t/^\circ C = 60.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	
NC3	0.19	0.11	0.09	0.13			BCL	5.95	5.91	5.17	4.76	3.91	3.41
NC4	0.26	0.12	0.03	0.24			PCL	10.10	9.50	8.25	7.03	5.76	4.71
NC5	0.18		0.15	0.22	0.13	0.16	CLH	18.49	15.95	13.24	10.37	8.23	6.63
NC6	0.38	0.21	0.15		0.12	0.15	CLO	67.14	47.12	33.67	23.66	17.24	12.71
NC7	0.68	0.55	0.49	0.64	0.74	0.32	D11	11.02	10.42	9.08	7.86	6.47	5.50
NC8	1.07	1.01	0.80	0.77	0.89	0.69	D12	59.11	46.05	35.47	27.57	21.33	16.89
NC9	2.24	1.81	1.30	1.30	1.28	0.95	MCH		6.20	6.01	5.76	5.03	4.35
C10	6.01	3.96	2.41	2.24	1.60	1.28	TCE	23.33	19.50	15.68	12.66	9.91	8.03
C11	15.02	8.10	4.71	3.46	2.82	1.81	CLB	118.04	87.98	65.28	48.82	36.24	27.86
CC5	0.82	0.64	0.70	0.85	0.68	0.57	ACT	34.34	27.81	22.16	17.77	14.21	11.57
CC6	1.06	1.22	1.26	1.46	1.14	1.19	MEK	46.49	36.81	28.68	22.57	17.50	14.15
CC7		2.90	3.05	3.27	2.84	2.69	THF	35.97	29.74	23.83	19.15	14.84	12.31
CC8	7.13	7.22	7.17	6.78	5.98	5.22	DOX	183.82	135.38	99.67	74.17	55.26	42.07
CHX		3.55	3.46	3.46	3.01	2.72	MAC	24.23	19.31	15.13	12.05	9.53	7.76
CHD		7.54	6.80	6.14	4.97	4.53	EAC	26.68	21.28	16.65	13.24	10.33	8.30
BNZ	19.03	17.46	14.68	12.38	10.07	8.16	PAC	38.75	30.35	23.14	17.86	13.69	10.87
TOL	32.48	28.73	22.25	17.96	14.03	11.20	NBA	63.49	47.20	34.84	26.02	19.41	14.97
EBZ	49.51	40.28	30.98	23.96	18.39	14.24	EOH	124.07	85.49	60.83	43.52	31.65	23.71
CL1	2.56	2.13	2.19	2.14	1.80	1.64	POH	188.00	127.34	88.03	62.40	44.30	32.56
CL2	22.59	18.25	14.49	11.78	9.38	7.67	BOH	314.61	203.01	137.55	93.68	64.74	46.53
CL3	29.36	24.76	19.91	16.08	12.60	10.17	AOH	522.40	324.80	211.71	140.42	94.43	66.10
CL4		5.51	5.32	5.19	4.54	3.97							

Table 9. Specific Retention Volume V_g of Various Probes on a PMA Column

	$V_g/(cm^3 g^{-1})$						$V_g/(cm^3 g^{-1})$						
	$t/^\circ C = 60.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	$t/^\circ C = 60.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	
NC3	0.52	0.49	0.72	0.68			BCL	55.09	43.76	34.63	27.93	22.38	18.11
NC4	1.32	1.27	1.52	1.45			PCL	112.77	85.42	65.00	50.74	39.37	30.98
NC5	2.28	2.66	2.86	2.51	2.33	2.00	CLH	227.13	165.05	119.45	90.07	67.96	52.03
NC6	5.47	5.65	5.37	4.88	4.20	3.62	CLO	899.31	593.22	397.19	278.94	198.68	142.65
NC7	12.13	11.59	10.27	8.97	7.44	6.39	D11	66.91	53.14	41.12	32.90	26.27	21.09
NC8	26.61	23.23	19.30	16.03	12.81	10.61	D12	230.11	166.79	121.30	92.34	70.13	53.95
NC9	57.47	45.88	35.64	28.43	22.20	17.65	MCH	60.85	52.71	42.35	34.60	27.91	22.47
C10	121.22	89.69	65.95	50.21	37.99	29.77	TCE	136.53	102.13	75.60	58.73	45.70	35.51
C11	250.11	171.58	120.60	88.49	65.00	49.56	CLB	609.78	432.72	311.00	228.78	168.56	124.54
CC5	7.35	7.85	7.23	6.76	5.84	4.91	ACT	60.62	46.37	35.61	28.85	22.95	18.54
CC6	14.68	15.47	14.38	12.85	10.96	9.26	MEK	110.92	82.37	61.65	48.43	37.56	29.46
CC7	51.35	47.02	39.96	33.46	27.24	22.17	THF	79.77	61.02	120.19	37.61	29.84	24.01
CC8	149.57	123.34	98.19	77.56	60.45	47.63	DOX	342.02	241.81	172.90	129.63	96.85	72.99
CHX	35.17	31.23	26.18	22.18	18.36	15.04	MAC	62.73	46.39	35.65	28.29	22.22	17.67
CHD	60.32	49.28	39.39	32.15	25.92	20.84	EAC	93.97	69.08	52.00	39.92	30.78	24.00
BNZ	111.80	85.89	65.98	52.11	40.82	32.33	PAC	175.20	124.98	90.84	68.27	51.31	38.95
TOL	224.53	163.82	121.15	92.39	70.28	54.02	NBA	344.65	236.31	166.26	120.89	88.39	65.45
EBZ	407.82	286.44	205.08	152.01	112.62	84.39	EOH	81.65	60.640	44.03	34.07	26.03	20.33
CL1	8.07	6.98	6.05	5.38	4.70	4.06	POH	177.19	121.389	86.61	64.94	48.57	36.74
CL2	75.68	57.00	43.96	34.85	27.64	21.95	BOH	358.30	244.098	168.88	122.98	89.31	65.69
CL3	138.93	103.32	77.45	59.99	46.17	36.24	AOH	711.77	472.929	321.32	226.55	159.51	114.13
CL4	54.07	46.82	38.33	31.51	25.32	20.44							

Table 10. Specific Retention Volume V_g of Various Probes on PEA

	$V_g/(cm^3 g^{-1})$					$V_g/(cm^3 g^{-1})$					
	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	$t/^\circ C = 70.0$	$t/^\circ C = 80.0$	$t/^\circ C = 90.0$	$t/^\circ C = 100.0$	$t/^\circ C = 110.0$	
NC3	1.59	1.73	1.74			NC9	134.11	94.85	70.49	52.12	41.23
NC4	3.41	2.89	2.58			C10	267.45	184.44	132.17	93.71	72.22
NC5	7.37	6.41	5.34	4.66	3.87	C11	536.80	357.79	245.65	168.09	125.34
NC6	15.56		10.15		7.13	CC5	18.60	15.31	12.77	10.35	8.70
NC7	32.10	25.19	20.10	16.15	13.25	CC6	37.88	30.02	24.58	19.75	16.34
NC8	65.83	49.04	37.54	28.90	23.56	CC7	107.88	81.21	63.63	49.28	39.86

Table 10 (Continued)

	$V_g(\text{cm}^3 \text{g}^{-1})$						$V_g(\text{cm}^3 \text{g}^{-1})$				
	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$
CC8	288.58	199.51	148.39	110.39	86.11	TCE	150.05	110.09	83.08	63.32	48.73
BNZ	118.56	88.57	68.39	52.21	41.61	CLB	613.85	425.56	305.80	218.26	162.85
TOL	240.58	179.06	129.01	94.78		ACT	49.51	37.92		23.19	20.64
EBZ	448.99	311.00	225.44	163.60	129.32	MEK	95.20	71.21	53.69	41.95	39.51
CL2	70.07	53.61	41.98	32.72		THF	79.26	60.84	46.50	36.97	
CL3	143.18	104.40	78.89	59.69	47.02	DOX	255.13	183.19	132.99	99.85	
CL4	80.14	60.73	47.33	37.01	30.13	MAC	51.45	35.89	29.15	24.18	19.50
BCL	70.33	53.93	42.35	32.97	26.86	EAC	83.04	61.42	45.86	36.23	28.42
PCL	145.46	107.86	81.07	61.11	49.37	PAC	162.15	115.91	84.05	63.81	48.97
CLH		209.33	152.38	112.48	85.38	NBA	329.30	221.51	158.08	115.80	86.76
CLO			533.15	366.12	260.48	EOH	66.81	49.80	38.03	29.09	23.03
D11	72.93	55.40	43.26	33.87		POH	147.75	102.18	75.64	56.29	43.45
D12	194.64	141.95	106.26	79.64	61.63	BOH	318.91	215.39	150.65	109.17	81.83
MCH	84.92	64.34	50.16	39.52	31.14						

Table 11. Specific Retention Volume V_g of Various Probes on PBMA

	$V_g(\text{cm}^3 \text{g}^{-1})$						$V_g(\text{cm}^3 \text{g}^{-1})$				
	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$
NC3	2.62	2.23	1.85			BCL	90.97	68.71	56.00	43.04	32.75
NC4	5.73	4.86	4.20			PCL	208.07	151.56	119.59	89.29	40.81
NC5	13.09	9.82	9.14	7.46	6.09	CLH	463.88	324.20	230.48	178.41	127.02
NC6	30.43	23.78	19.60	15.70	12.52	CLO	2272.02	1463.36	953.25	696.52	460.69
NC7	69.68	52.61	40.89	31.78	25.06	D11	72.11	54.81	44.80	34.71	26.83
NC8	153.63	111.60	83.38	63.51	48.62	D12	166.13	122.08	96.04	73.01	54.54
NC9	338.45	236.01	173.33	124.82	92.34	MCH	96.17	73.67	56.83	46.86	36.02
C10	744.65	496.89	351.72	243.81	173.59	TCE	180.38	131.04	97.58	77.91	58.22
C11	1628.94	1044.87	709.32	474.58	326.15	CLB	700.02	489.95	346.67	266.64	190.25
CC5	29.05	23.57	19.43	15.90	12.72	ACT	34.49	26.91	21.28	17.91	14.11
CC6	63.78	50.75	41.38	33.13	26.72	MEK	78.83	59.28	45.47	36.79	28.65
CC7	201.89	152.26	119.31	90.57	69.01	THF	80.13	61.03	44.96	38.64	29.91
CC8	559.66	405.10	297.11	220.50	164.55	DOX	202.27	145.39	108.58	86.48	64.85
CHX	90.00	69.68	55.90	44.57	34.74	MAC	37.99	29.18	22.65	18.82	14.60
CHD	102.28	78.54	62.60	49.73	37.61	EAC	69.84	51.75	39.15	31.92	24.38
BNZ	128.34	96.91	76.09	57.62	44.99	PAC	152.81	108.79	80.28	63.57	47.05
TOL	290.08	209.76	159.72	116.76	87.68	NBA	344.79	235.40	167.02	128.80	92.53
EBZ	594.51	413.53	290.80	216.46	157.11	EOH	44.93	33.23	24.65	20.18	15.36
CL1	8.13	6.95	5.83	5.39	4.68	POH	112.13	79.13	57.87	45.69	34.07
CL2	59.16	45.69	36.82	28.92	22.28	BOH	270.86	182.49	128.92	99.43	70.77
CL3	139.65	102.34	79.78	61.55	45.66	AOH	633.04	410.05	279.68	208.21	142.25
CL4	97.24	74.44	61.08	47.66	36.77						

Table 12. Flory-Huggins Interaction Parameters χ_{12} for PEE

	χ_{12} (unitless)							χ_{12} (unitless)					
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$
NC3	0.454	0.494	0.441	0.366			BCL	0.548	0.525	0.508	0.485	0.472	0.452
NC4	0.396	0.416	0.361	0.340			PCL	0.465	0.436	0.420	0.395	0.380	0.355
NC5	0.349	0.360	0.338	0.345	0.324	0.326	CLH	0.425	0.401	0.392	0.375	0.369	0.353
NC6	0.302	0.304	0.293	0.286	0.285	0.287	CLO	0.402	0.373	0.354	0.340	0.336	0.330
NC7	0.271	0.272	0.255	0.255	0.257	0.260	D11	0.805	0.762	0.731	0.691	0.662	0.633
NC8	0.252	0.253	0.234	0.238	0.241	0.243	D12	1.122	1.071	1.032	0.983	0.953	0.912
NC9	0.243	0.214	0.220	0.228	0.228	0.233	MCH	0.416	0.381	0.369	0.333	0.319	0.293
C10	0.236	0.210	0.212	0.218	0.221	0.223	TCE	0.405	0.387	0.383	0.362	0.356	0.343
C11	0.218	0.203	0.190	0.200	0.217		CLB	0.603	0.572	0.552	0.529	0.514	0.494
CC5	0.196	0.193	0.173	0.184	0.196	0.177	ACT	2.156	2.043	1.899	1.805	1.741	1.627
CC6	0.155	0.147	0.129	0.136	0.137	0.135	MEK	1.628	1.552	1.488	1.418	1.369	1.295
CC7	0.078	0.074	0.068	0.064	0.068	0.060	THF	0.647	0.614	0.587	0.557	0.541	0.505
CC8	0.034	0.033	0.032	0.032	0.037	0.029	DOX	1.351	1.299	1.237	1.180	1.148	1.083
CHX	0.211	0.203	0.194	0.192	0.189	0.181	MAC	1.646	1.574	1.497	1.442	1.403	1.325
CHD	0.365	0.352	0.336	0.323	0.306		EAC	1.346	1.293	1.234	1.183	1.154	1.094
BNZ	0.579	0.550	0.524	0.499	0.484	0.460	PAC	1.153	1.097	1.047	0.999	0.966	0.916
TOL	0.490	0.468	0.443	0.431	0.422	0.401	NBA	1.004	0.958	0.917	0.880	0.851	0.808
EBZ	0.458	0.434	0.412	0.400	0.391	0.373	EOH	3.813	3.628	3.231	3.072	3.066	2.716
CL1	0.897	0.863	0.709	0.736	0.621	0.662	POH	3.213	3.014	2.770	2.602	2.457	2.252
CL2	0.996	0.953	0.888	0.866	0.825	0.777	BOH	2.964	2.748	2.534	2.358	2.209	2.018
CL3	0.638	0.626	0.606	0.607	0.609	0.594	AOH	2.720	2.470	2.284	2.124	1.984	1.832
CL4	0.268	0.251	0.234	0.230	0.226	0.211							

Table 13. Flory-Huggins Interaction Parameters χ_{12} for PP1

	χ_{12}						χ_{12}				
	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
NC3	0.526	0.465	0.719	0.772	0.502	BCL	0.573	0.594	0.566	0.480	0.471
NC4	0.508	0.427	0.579	0.594	0.484	PCL	0.499	0.459	0.486	0.412	0.338
NC5	0.415	0.401	0.430	0.696	0.386	CLH	0.429	0.424	0.428	0.358	0.298
NC6	0.338	0.312	0.360	0.330	0.267	CLO	0.379	0.348	0.366	0.327	0.235
NC7	0.285	0.262	0.307	0.275	0.388	D11	0.837	0.782	0.797	0.721	0.673
NC8	0.255	0.236	0.271	0.234	0.163	D12	1.125	1.065	1.067	0.991	0.937
NC9	0.327	0.203	0.248	0.209	0.132	MCH	0.461	0.429	0.438	0.367	0.299
C10	0.192	0.175	0.230	0.184	0.079	TCE	0.445	0.439	0.440	0.390	0.334
C11	0.199	0.132	0.217	0.171	0.090	CLB	0.618	0.609	0.604	0.575	0.463
CC5	0.252	0.242	0.281	0.256	0.222	ACT	2.189	1.911	1.787	1.770	1.620
CC6	0.202	0.192	0.145	0.179	0.138	MEK	1.602	1.531	1.496	1.351	1.310
CC7	0.125	0.110	0.143	0.100	0.033	THF	0.683	0.641	0.641	0.586	0.532
CC8	0.101	0.090	0.100	0.057	-0.009	DOX	1.356	1.281	1.259	1.171	1.087
CHX	0.263	0.250	0.277	0.223	0.188	MAC	1.697	1.502	1.414	1.379	1.301
CHD	0.416	0.397	0.420	0.354	0.322	EAC	1.344	1.270	1.273	1.175	1.138
BNZ	0.606	0.588	0.592	0.520	0.467	PAC	1.134	1.074	1.065	0.987	0.860
TOL	0.512	0.480	0.489	0.427	0.363	NBA	0.981	0.914	0.929	0.858	0.761
EBZ	0.467	0.435	0.410	0.373	0.328	EOH	3.540	3.207	2.923	2.776	2.740
CL1	0.841	0.802	0.802	0.645	0.665	POH	3.130	2.793	2.588	2.392	2.205
CL2	1.044	0.938	0.948	0.851	0.954	BOH	2.810	2.600	2.430	2.244	2.020
CL3	0.646	0.622	0.597	0.531	0.471	AOH	2.514	2.326	2.188	2.028	1.798
CL4	0.363	0.329	0.345	0.277	0.232						

Table 14. Flory-Huggins Interaction Parameters χ_{12} for PDMS

	χ_{12}							χ_{12}					
	$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
NC3	0.284	0.222	0.261	0.202			BCL	0.581	0.567	0.546	0.533	0.504	0.482
NC4	0.312	0.276	0.295	0.263			PCL	0.580	0.563	0.540	0.519	0.487	0.460
NC5	0.350	0.327	0.333	0.323	0.277	0.299	CLH	0.618	0.605	0.584	0.567	0.543	0.526
NC6	0.387	0.359	0.365	0.349	0.321	0.323	CLO	0.738	0.715	0.689	0.668	0.645	0.627
NC7	0.432	0.403	0.406	0.389	0.365	0.355	D11	0.733	0.705	0.676	0.649	0.611	0.615
NC8	0.489	0.455	0.458	0.439	0.412	0.408	D12	1.105	1.068	1.034	1.002	0.954	0.950
NC9	0.554	0.517	0.513	0.492	0.465	0.458	MCH	0.459	0.441	0.422	0.406	0.372	0.377
C10	0.555	0.558	0.557	0.548	0.522	0.508	TCE	0.599	0.587	0.576	0.565	0.539	0.543
C11	0.734	0.686	0.642	0.612	0.580	0.566	CLB	0.866	0.841	0.821	0.798	0.778	0.773
CC5	0.352	0.324	0.329	0.331	0.296	0.316	ACT	1.635	1.544	1.452	1.373	1.281	1.277
CC6	0.427	0.395	0.396	0.387	0.354	0.357	MEK	1.284	1.235	1.165	1.134	1.077	1.065
CC7	0.512	0.482	0.466	0.460	0.429	0.422	THF	0.555	0.539	0.526	0.502	0.473	0.485
CC8	0.585	0.566	0.552	0.539	0.508	0.501	DOX	1.200	1.158	1.110	1.078	1.031	1.027
CHX	0.430	0.422	0.405	0.396	0.378	0.366	MAC	1.175	1.128	1.077	1.043	0.983	0.986
CHD	0.520	0.510	0.489	0.480	0.460	0.443	EAC	0.944	0.913	0.883	0.855	0.812	0.814
BNZ	0.680	0.658	0.641	0.616	0.581	0.581	PAC	0.842	0.812	0.784	0.753	0.720	0.710
TOL	0.690	0.672	0.663	0.635	0.606	0.607	NBA	0.785	0.763	0.738	0.714	0.688	0.681
EBZ	0.718	0.699	0.678	0.659	0.635	0.632	EOH	3.072	2.842	2.658	2.469	2.269	2.259
CL1	0.631	0.597	0.558	0.500	0.402	0.394	POH	2.679	2.494	2.356	2.173	2.000	1.922
CL2	0.822	0.788	0.761	0.738	0.688	0.714	BOH	2.534	2.347	2.200	2.033	1.879	1.780
CL3	0.654	0.651	0.660	0.658	0.643	0.678	AOH	2.326	2.165	2.017	1.883	1.754	1.662
CL4	0.427	0.417	0.414	0.399	0.378	0.390							

Table 15. Flory-Huggins Interaction Parameters χ_{12} for PCL

	χ_{12}						χ_{12}				
	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
NC3	1.281	1.248	1.286			CL1	0.198	0.184	0.144	0.194	0.190
NC4	1.238	1.268	1.145			CL2	-0.338	-0.302	-0.273	-0.216	-0.197
NC5	1.274	1.255	1.183	1.216	1.205	CL3	-0.594	-0.537	-0.481	-0.395	-0.346
NC6	1.319	1.291	1.234	1.227	1.197	CL4	0.237	0.241	0.249	0.280	0.288
NC7	1.380	1.332	1.287	1.263	1.225	BCL	0.362	0.356	0.349	0.377	0.370
NC8	1.444	1.396	1.347	1.318	1.269	PCL	0.379	0.365	0.351	0.369	0.349
NC9	1.527	1.474	1.420	1.386	1.333	CLH	0.449	0.444	0.425	0.443	0.426
C10	1.589	1.539	1.498	1.456	1.398	CLO	0.607	0.597	0.568	0.580	0.556
C11	1.702	1.640	1.579	1.526	1.476	D11	-0.067	-0.046	-0.038	0.011	0.015
CC5	0.887	0.873	0.825	0.829	0.823	D12	-0.197	-0.168	-0.152	-0.101	-0.087
CC6	0.989	0.953	0.916	0.896	0.870	MCH	0.064	0.072	0.070	0.101	0.097
CC7	0.953	0.916	0.871	0.843	0.818	TCE	-0.027	-0.000	0.034	0.054	0.068
CC8	0.958	0.917	0.874	0.853	0.822	CLB	-0.125	-0.105	-0.085	-0.053	-0.044
CHX	0.636	0.621	0.595	0.589	0.584	ACT	0.545	0.520	0.512	0.503	0.486
CHD	0.352	0.350	0.345	0.352	0.351	MEK	0.380	0.372	0.382	0.382	0.369
BNZ	0.031	0.044	0.047	0.072	0.078	THF	0.128	0.132	0.140	0.146	0.133
TOL	0.057	0.072	0.073	0.096	0.110	DOX	0.109	0.120	0.137	0.152	0.148
EBZ	0.157	0.163	0.160	0.178	0.186	MAC	0.389	0.393	0.406	0.424	0.419

Table 15 (Continued)

	χ_{12}						χ_{12}				
	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
EAC	0.356	0.364	0.377	0.390	0.388	POH	0.894	0.835	0.780	0.736	0.674
PAC	0.339	0.339	0.346	0.352	0.345	BOH	0.779	0.714	0.652	0.608	0.544
NBA	0.314	0.319	0.325	0.333	0.325	AOH	0.607	0.556	0.510	0.479	0.433
EOH	1.168	1.100	1.049	0.994	0.981						

Table 16. Flory-Huggins Interaction Parameters χ_{12} for PECH

	χ_{12}							χ_{12}					
	$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
NC3	2.021	2.109	1.612	1.978			BCL	0.692	0.676	0.660	0.640	0.620	0.603
NC4	1.934	1.812	1.717	1.668			PCL	0.763	0.741	0.711	0.686	0.682	0.658
NC5	2.058	1.943	1.796	1.782	1.675	1.680	CLH	0.876	0.854	0.823	0.798	0.761	0.737
NC6	2.020	1.936	1.849	1.789	1.733	1.642	CLO	1.148	1.116	1.076	1.023	0.979	0.943
NC7	2.114	2.021	1.928	1.866	1.779	1.702	D11	0.360	0.369	0.358	0.362	0.349	0.339
NC8	2.244	2.143	2.051	1.970	1.887	1.803	D12	0.156	0.182	0.191	0.206	0.205	0.213
NC9	2.386	2.273	2.176	2.082	1.994	1.914	MCH	0.544	0.513	0.494	0.481	0.456	0.432
C10	2.504	2.384	2.284	2.200	2.102	2.012	TCE	0.545	0.553	0.550	0.536	0.518	0.503
C11	2.664	2.540	2.430	2.325	2.218	2.125	CLB	0.227	0.244	0.250	0.242	0.235	0.237
CC5	1.368	1.303	1.252	1.202	1.179	1.132	ACT	0.292	0.299	0.298	0.292	0.275	0.267
CC6	1.470	1.389	1.320	1.270	1.222	1.157	MEK	0.164	0.183	0.194	0.199	0.194	0.189
CC7	1.443	1.361	1.294	1.236	1.176	1.122	THF	-0.026	-0.005	0.006	0.015	0.010	0.015
CC8	1.458	1.378	1.311	1.247	1.184	1.133	DOX	-0.056	-0.020	0.000	0.019	0.026	0.050
CHX	1.019	0.967	0.931	0.892	0.861	0.827	MAC	0.335	0.348	0.362	0.367	0.359	0.372
CHD	0.643	0.610	0.598	0.573	0.558	0.543	EAC	0.314	0.336	0.342	0.350	0.344	0.357
BNZ	0.250	0.238	0.234	0.237	0.234	0.232	PAC	0.317	0.333	0.334	0.333	0.323	0.332
TOL	0.310	0.299	0.297	0.299	0.292	0.294	NBA	0.341	0.360	0.358	0.357	0.347	0.350
EBZ	0.474	0.456	0.445	0.440	0.425	0.423	EOH	1.799	1.697	1.611	1.522	1.485	1.382
CL1	0.523	0.481	0.365	0.354	0.316	0.314	POH	1.582	1.489	1.385	1.294	1.194	1.114
CL2	0.163	0.170	0.166	0.184	0.190	0.187	BOH	1.513	1.411		1.199	1.098	1.028
CL3	0.175	0.191	0.219	0.252	0.278	0.273	AOH	1.391	1.284		1.098	1.008	0.940
CL4	0.789	0.753	0.729	0.709	0.686	0.658							

Table 17. Flory-Huggins Interaction Parameters χ_{12} for PHEA

	χ_{12}							χ_{12}					
	$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
NC7	5.625	5.498	5.306	4.742	4.329	4.404	CLH	3.683	3.432	3.253	3.149	3.062	2.973
NC8	6.044	5.711	5.594	5.298	4.846	4.804	CLO	4.137	3.996	3.878	3.800	3.721	3.649
NC9	6.174	5.953	5.884	5.509	5.182	5.153	D11	2.027	1.800	1.678	1.575	1.544	1.489
C10	6.043	5.979	6.032	5.704	5.651	5.507	D12	1.264	1.196	1.166	1.140	1.142	1.130
C11	6.014	6.103	6.158	6.005	5.788	5.826	MCH		2.645	2.400	2.178	2.069	1.983
CC5	4.267	4.253	3.922	3.503	3.518	3.490	TCE	2.181	2.042	1.967	1.901	1.889	1.853
CC6	4.879	4.435	4.125	3.713	3.717	3.442	CLB	1.970	1.881	1.828	1.784	1.775	1.743
CC7		4.652	4.274	3.891	3.742	3.522	ACT	0.981	0.899	0.857	0.821	0.807	0.786
CC8	5.150	4.730	4.362	4.063	3.861	3.684	MEK	1.259	1.175	1.132	1.091	1.087	1.051
CHX		3.496	3.240	2.971	2.863	2.730	THF	1.152	1.042	0.989	0.946	0.959	0.915
CHD		2.728	2.551	2.386	2.355	2.215	DOX	0.757	0.705	0.685	0.669	0.678	0.679
BNZ	2.173	1.948	1.836	1.736	1.694	1.667	MAC	1.278	1.208	1.181	1.150	1.149	1.128
TOL	2.489	2.259	2.190	2.097	2.060	2.015	EAC	1.661	1.562	1.512	1.459	1.449	1.420
EBZ	2.841	2.652	2.553	2.465	2.414	2.367	PAC	2.012	1.888	1.822	1.761	1.734	1.685
CL1	1.475	1.473	1.273	1.126	1.155	1.118	NBA	2.281	2.170	2.101	2.039	2.009	1.959
CL2	1.003	0.950	0.938	0.913	0.928	0.927	EOH	0.812	0.780	0.749	0.728	0.718	0.724
CL3	1.313	1.215	1.191	1.175	1.214	1.232	POH	0.985	0.927	0.889	0.845	0.833	0.801
CL4		2.903	2.665	2.429	2.323	2.229	BOH	1.216	1.153	1.090	1.045	1.025	0.985
BCL	3.119	2.819	2.671	2.486	2.437	2.342	AOH	1.356	1.306	1.255	1.214	1.202	1.170
PCL	3.428	3.134	2.947	2.794	2.705	2.629							

Table 18. Flory-Huggins Interaction Parameters χ_{12} for PMA

	χ_{12}							χ_{12}					
	$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$		$t/^{\circ}\text{C} = 60.0$	$t/^{\circ}\text{C} = 70.0$	$t/^{\circ}\text{C} = 80.0$	$t/^{\circ}\text{C} = 90.0$	$t/^{\circ}\text{C} = 100.0$	$t/^{\circ}\text{C} = 110.0$
NC3	2.401	2.325	1.793	1.738			CC6	2.316	1.960	1.750	1.603	1.520	1.460
NC4	2.392	2.233	1.870	1.753			CC7	2.204	1.934	1.762	1.632	1.550	1.483
NC5	2.731	2.336	2.037	1.958	1.839	1.812	CC8	2.175	1.959	1.807	1.693	1.616	1.544
NC6	2.731	2.407	2.187	2.034	1.955	1.885	CHX	1.581	1.390	1.278	1.180	1.123	1.088
NC7	2.808	2.516	2.321	2.168	2.085	1.983	CHD	1.023	0.918	0.857	0.798	0.770	0.757
NC8	2.895	2.645	2.470	2.326	2.244	2.142	BNZ	0.471	0.423	0.396	0.366	0.362	0.359
NC9	3.000	2.789	2.636	2.492	2.394	2.297	TOL	0.624	0.586	0.557	0.526	0.517	0.511
C10	3.107	2.925	2.800	2.659	2.553	2.434	EBZ	0.801	0.758	0.724	0.685	0.670	0.658
C11	3.271	3.117	2.975	2.831	2.716	2.587	CL1	0.387	0.341	0.304	0.253	0.233	0.230
CC5	2.140	1.811	1.649	1.491	1.430	1.407	CL2	-0.137	-0.120	-0.109	-0.105	-0.085	-0.056

Table 18 (Continued)

	χ_{12}							χ_{12}					
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$		$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	
	60.0	70.0	80.0	90.0	100.0	110.0		60.0	70.0	80.0	90.0	100.0	110.0
CL3	-0.222	-0.205	-0.175	-0.156	-0.111	-0.075	MEK	0.459	0.437	0.428	0.400	0.392	0.388
CL4	0.986	0.831	0.752	0.692	0.671	0.658	THF	0.425	0.392	0.428	0.343	0.330	0.316
BCL	0.963	0.885	0.832	0.784	0.761	0.740	DOX	0.205	0.193	0.195	0.184	0.186	0.198
PCL	1.085	1.005	0.944	0.884	0.850	0.815	MAC	0.396	0.400	0.386	0.368	0.370	0.375
CLH	1.243	1.163	1.114	1.055	1.018	0.982	EAC	0.471	0.453	0.434	0.427	0.425	0.428
CLO	1.611	1.531	1.469	1.400	1.347	1.302	PAC	0.572	0.540	0.515	0.493	0.481	0.478
D11	0.292	0.239	0.230	0.211	0.210	0.214	NBA	0.658	0.627	0.599	0.577	0.562	0.554
D12	-0.026	-0.022	-0.001	-0.001	0.019	0.039	EOH	1.300	1.192	1.133	1.046	0.983	0.949
MCH	0.731	0.573	0.509	0.452	0.426	0.410	POH	1.113	1.044	0.965	0.879	0.810	0.752
TCE	0.484	0.454	0.456	0.434	0.430	0.436	BOH	1.155	1.037	0.943	0.848	0.773	0.711
CLB	0.397	0.356	0.328	0.313	0.307	0.316	AOH	1.121	0.999	0.896	0.811	0.747	0.695
ACT	0.482	0.456	0.445	0.408	0.397	0.384							

Table 19. Flory-Huggins Interaction Parameters χ_{12} for PEA

	χ_{12}						χ_{12}				
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$		$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$
	70.0	80.0	90.0	100.0	110.0		70.0	80.0	90.0	100.0	110.0
NC3	1.169	0.938	0.797			PCL	0.577	0.551	0.532	0.525	0.480
NC4	1.318	1.296	1.232			CLH		0.646	0.619	0.596	0.579
NC5	1.401	1.316	1.288	1.225	1.229	CLO			0.838	0.817	0.794
NC6	1.483		1.392		1.296	D11	0.012	0.027	0.027	0.042	
NC7	1.585	1.517	1.451	1.396	1.345	D12	-0.085	-0.061	-0.049	-0.019	0.004
NC8	1.691	1.631	1.566	1.515	1.436	MCH	0.200	0.203	0.192	0.191	0.209
NC9	1.814	1.753	1.676	1.628	1.543	TCE	0.163	0.179	0.181	0.195	0.220
C10	1.926	1.849	1.783	1.736	1.645	CLB	0.094	0.108	0.103	0.129	0.140
C11	2.069	1.982	1.901	1.850	1.753	ACT	0.507	0.506		0.508	0.411
CC5	1.031	0.984	0.938	0.935	0.914	MEK	0.400	0.399	0.403	0.392	0.218
CC6	1.148	1.101	1.038	1.010	0.974	THF	0.215	0.203	0.207	0.191	
CC7	1.189	1.143	1.076	1.036	0.983	DOX	0.239	0.244	0.254	0.255	
CC8	1.199	1.189	1.132	1.092	1.041	MAC	0.402	0.491	0.442	0.392	0.394
BNZ	0.183	0.187	0.176	0.191	0.188	EAC	0.365	0.370	0.379	0.358	0.363
TOL	0.289	0.259	0.281	0.301		PAC	0.371	0.369	0.369	0.352	0.347
EBZ	0.396	0.400	0.380	0.379	0.321	NBA	0.394	0.409	0.391	0.379	0.370
CL2	-0.240	-0.217	-0.203	-0.172		EOH	1.211	1.129	1.046	1.016	0.960
CL3	-0.478	-0.426	-0.394	-0.351	-0.322	POH	0.949	0.901	0.814	0.756	0.690
CL4	0.384	0.388	0.378	0.379	0.365	BOH	0.869	0.797	0.725	0.658	0.589
BCL	0.496	0.479	0.455	0.452	0.432						

Table 20. Flory-Huggins Interaction Parameters χ_{12} for PBMA

	χ_{12}						χ_{12}				
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$		$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$
	70.0	80.0	90.0	100.0	110.0		70.0	80.0	90.0	100.0	110.0
NC3	0.739	0.768	0.830			BCL	0.297	0.298	0.232	0.249	0.292
NC4	0.860	0.842	0.814			PCL	0.258	0.249	0.171	0.174	0.258
NC5	0.883	0.950	0.807	0.814	0.833	CLH	0.273	0.268	0.259	0.195	0.235
NC6	0.867	0.849	0.787	0.777	0.786	CLO	0.331	0.319	0.314	0.232	0.275
NC7	0.866	0.838	0.794	0.775	0.761	D11	0.079	0.093	0.046	0.074	0.119
NC8	0.899	0.867	0.821	0.784	0.763	D12	0.127	0.144	0.103	0.122	0.174
NC9	0.934	0.899	0.827	0.808	0.785	MCH	0.117	0.107	0.100	0.049	0.083
C10	0.951	0.916	0.855	0.835	0.814	TCE	0.031	0.057	0.071	0.038	0.087
C11	1.009	0.970	0.892	0.868	0.846	CLB	0.019	0.026	0.035	-0.011	0.038
CC5	0.646	0.616	0.579	0.569	0.597	ACT	0.898	0.876	0.852	0.787	0.803
CC6	0.687	0.639	0.577	0.556	0.543	MEK	0.627	0.619	0.602	0.555	0.561
CC7	0.620	0.576	0.504	0.490	0.491	THF	0.265	0.262	0.303	0.213	0.242
CC8	0.590	0.542	0.494	0.463	0.448	DOX	0.517	0.520	0.499	0.441	0.462
CHX	0.475	0.450	0.399	0.378	0.396	MAC	0.745	0.737	0.731	0.678	0.711
CHD	0.332	0.317	0.276	0.261	0.312	EAC	0.588	0.590	0.585	0.530	0.558
BNZ	0.165	0.163	0.131	0.159	0.173	PAC	0.485	0.487	0.469	0.408	0.434
TOL	0.158	0.160	0.122	0.151	0.171	NBA	0.394	0.404	0.391	0.326	0.353
EBZ	0.172	0.175	0.180	0.157	0.181	EOH	1.638	1.567	1.507	1.403	1.375
CL1	0.333	0.314	0.319	0.238	0.235	POH	1.269	1.208	1.131	1.011	0.972
CL2	-0.013	0.003	-0.016	0.013	0.074	BOH	1.079	1.019	0.936	0.805	0.782
CL3	-0.396	-0.347	-0.350	-0.320	-0.237	AOH	0.852	0.807	0.735	0.620	0.620
CL4	0.244	0.239	0.174	0.182	0.216						

Table 21. Parameters B_{12} for PEE

	$B_{12}/(\text{J}/\text{cm}^3)$							$B_{12}/(\text{J}/\text{cm}^3)$					
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$		$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	
	60.0	70.0	80.0	90.0	100.0	110.0		60.0	70.0	80.0	90.0	100.0	110.0
NC3	12.38	13.23	11.54	9.24			NC5	7.86	8.19	7.76	7.97	7.52	7.58
NC4	9.98	10.51	9.10	8.52			NC6	6.03	6.15	6.02	5.93	5.97	6.05

Table 21 (Continued)

	$B_{12}/(\text{J}/\text{cm}^3)$						$B_{12}/(\text{J}/\text{cm}^3)$						
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC7	4.86	4.96	4.72	4.79	4.88	5.00	CLH	8.21	7.90	7.85	7.64	7.64	7.40
NC8	4.09	4.19	3.93	4.07	4.16	4.26	CLO	6.29	5.95	5.75	5.63	5.66	5.64
NC9	3.60	3.64	3.38	3.56	3.61	3.75	D11	25.04	24.05	23.38	22.35	21.65	20.88
C10	3.22	2.92	2.99	3.13	3.22	3.30	D12	37.52	36.40	35.63	34.43	33.84	32.78
C11		2.80	2.66	2.53	2.71	2.99	MCH	10.99	10.21	10.02	9.18	8.88	8.24
CC5	5.47	5.45	4.96	5.33	5.73	5.20	TCE	11.88	11.56	11.61	11.14	11.10	10.81
CC6	3.77	3.63	3.26	3.46	3.54	3.52	CLB	15.75	15.23	14.98	14.60	14.42	14.07
CC7	1.71	1.64	1.54	1.49	1.59	1.41	ACT	76.63	73.60	69.23	66.51	64.74	60.95
CC8	0.68	0.67	0.67	0.67	0.78	0.63	MEK	47.82	46.30	45.02	43.49	42.48	40.61
CHX	5.49	5.36	5.21	5.22	5.21	5.05	THF	20.74	19.90	19.22	18.41	18.00	16.92
CHD	10.14	9.94	9.62		9.50	9.10	DOX	43.46	42.63	41.40	40.21	39.83	38.17
BNZ	17.15	16.58	16.02	15.47	15.20	14.60	MAC	54.11	52.43	50.47	49.15	48.23	45.89
TOL	12.21	11.89	11.43	11.30	11.23	10.82	EAC	36.02	35.09	33.94	32.92	32.46	31.04
EBZ	9.94	9.60	9.29	9.17	9.09	8.82	PAC	26.37	25.51	24.69	23.90	23.38	22.43
CL1	40.17	38.52	31.41	32.20	26.57	27.32	NBA	20.12	19.53	19.00	18.51	18.16	17.48
CL2	40.58	39.34	37.12	36.60	35.15	33.35	EOH	172.81	167.23	151.28	145.91	147.56	132.27
CL3	20.82	20.73	20.34	20.62	20.91	20.60	POH	113.97	108.80	101.66	96.99	92.88	86.25
CL4	7.30	6.97	6.58	6.56	6.54	6.16	BOH	86.13	81.32	76.32	72.19	68.68	63.63
BCL	13.81	13.47	13.22	12.80	12.61	12.22	AOH	66.92	61.91	58.25	55.09	52.24	48.95
PCL	10.17	9.70	9.50	9.09	8.86	8.40							

Table 22. Parameters B_{12} for PPI

	$B_{12}/(\text{J}/\text{cm}^3)$					$B_{12}/(\text{J}/\text{cm}^3)$					
	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC3	14.09	12.16	16.93	18.60		BCL	14.69	15.45	14.19	12.82	13.15
NC4	12.83	10.77	13.60	14.69		PCL	11.10	10.40	10.24	9.62	
NC5	9.43	9.20	9.27		9.42	CLH	8.45	8.62	8.08	7.40	6.44
NC6	6.85	6.41	6.95	6.92	6.05	CLO	6.05	5.66	5.61	5.52	4.26
NC7	5.20	4.85	5.29	5.21	4.64	D11	26.44	25.00	25.01	22.80	22.94
NC8	4.21	3.96	4.20	4.05	3.19	D12	38.23	36.79	36.66	34.53	34.64
NC9	4.94	3.13	3.53	3.31	2.50	MCH	12.36	11.65	11.63	10.21	9.44
C10	2.67	2.47	2.97	2.69	1.16	TCE	13.29	13.30	12.96	12.05	11.39
C11	2.56	1.73	2.57	2.32	1.51	CLB	16.46	16.68	15.77	15.10	13.41
CC5	7.12	6.91	7.18	7.49	6.87	ACT	78.84	69.66	71.35	63.85	60.72
CC6	5.00	4.82		4.63	3.93	MEK	47.80	46.34	45.77	42.22	42.73
CC7	2.78	2.49	2.66	2.34	1.14	THF	22.15	21.00	20.12	18.41	18.27
CC8	2.04	2.05	1.54	1.22	0.15	DOX	44.50	42.86	42.57	39.75	39.78
CHX	6.96	6.70	6.42	6.16	5.21	MAC	56.54	50.66	48.18	47.15	45.07
CHD	11.75	11.38	11.57	10.43	10.28	EAC	36.47	34.94	34.92	32.13	33.23
BNZ	18.26	17.98	17.31	16.32	15.11	PAC	26.36	25.33	24.95	23.30	21.06
TOL	13.00	12.40	12.17	11.37	10.29	NBA	20.01	18.95	19.09	17.91	17.01
EBZ	10.33	9.79		8.67	8.16	EOH	163.19	150.13	156.18	143.76	133.44
CL1	37.53	35.51	34.29	27.61	29.46	POH	112.98	102.52	99.74	93.35	84.44
CL2	43.10	39.21	38.77	36.28	41.69	BOH	83.16	78.30	73.61	69.37	64.50
CL3	21.39	20.89	20.28	18.25	21.52	AOH	62.99	59.33	56.11	52.34	48.72
CL4	10.07	9.26	9.21	7.99	7.46						

Table 23. Parameters B_{12} for PDMS

	$B_{12}/(\text{J}/\text{cm}^3)$						$B_{12}/(\text{J}/\text{cm}^3)$						
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC3	7.75	5.95	6.82	5.11	5.23	2.43	CL3	21.34	21.56	22.17	22.37	22.06	23.49
NC4	7.86	6.96	7.44	6.60	6.30	6.38	CL4	11.65	11.55	11.66	11.38	10.91	11.38
NC5	7.86	7.43	7.63	7.46	6.43	6.95	BCL	14.65	14.54	14.22	14.07	13.48	13.02
NC6	7.73	7.28	7.49	7.24	6.72	6.81	PCL	12.69	12.54	12.22	11.93	11.36	10.88
NC7	7.74	7.34	7.51	7.29	6.93	6.82	CLH	11.93	11.91	11.71	11.55	11.23	11.04
NC8	7.95	7.51	7.69	7.49	7.13	7.15	CLO	11.55	11.41	11.21	11.05	10.86	10.72
NC9	8.21	7.81	7.88	7.68	7.38	7.38	D11	22.82	22.25	21.64	21.00	19.99	20.29
C10	7.56	7.74	7.87	7.87	7.62	7.53	D12	36.93	36.32	35.71	35.12	33.89	34.15
C11	9.26	8.81	8.40	8.15	7.85	7.79	MCH	12.11	11.81	11.47	11.18	10.36	10.61
CC5	9.80	9.16	9.41	9.56	8.64	9.31	TCE	17.59	17.54	17.47	17.35	16.78	17.11
CC6	10.42	9.79	9.98	9.87	9.15	9.33	CLB	22.64	22.39	22.26	22.02	21.80	22.00
CC7	11.23	10.76	10.58	10.59	10.02	9.98	ACT	58.09	55.60	52.92	50.58	47.64	47.84
CC8	11.61	11.45	11.37	11.31	10.83	10.85	MEK	37.72	36.85	35.25	34.78	33.42	33.40
CHX	11.18	11.15	10.87	10.78	10.41	10.19	THF	17.79	17.48	17.23	16.57	15.74	16.22
CHD	14.43	14.39	14.02	13.95	13.55	13.20	DOX	38.59	38.02	37.15	36.76	35.74	36.21
BNZ	20.16	19.82	19.60	19.08	18.25	18.46	MAC	38.64	37.60	36.33	35.55	33.79	34.14
TOL	17.20	17.05	17.12	16.66	16.13	16.39	EAC	25.27	24.79	24.28	23.79	22.85	23.08
EBZ	15.60	15.46	15.28	15.10	14.78	14.92	PAC	19.25	18.87	18.49	18.00	17.44	17.39
CL1	28.28	26.63	24.72	21.84	17.20	16.28	NBA	15.73	15.56	15.29	15.03	14.69	14.74
CL2	33.48	32.53	31.81	31.18	29.34	30.64	EOH	139.23	130.99	124.44	117.26	109.21	110.03

Table 23 (Continued)

	$B_{12}/(\text{J}/\text{cm}^3)$						$B_{12}/(\text{J}/\text{cm}^3)$						
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
POH	95.01	90.05	86.46	80.98	75.61	73.60	OH	57.22	54.26	51.45	48.82	46.18	44.41
BOH	73.63	69.48	66.26	62.25	58.41	56.13							

Table 24. Parameters B_{12} for PCL

	$B_{12}/(\text{J}/\text{cm}^3)$					$B_{12}/(\text{J}/\text{cm}^3)$					
	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC3	34.33	32.61	32.45			BCL	9.28	9.27	9.21	10.08	10.00
NC4	31.27	31.96	28.71			PCL	8.44	8.27	8.08	8.60	8.24
NC5	28.97	28.78	27.31	28.21	28.00	CLH	8.84	8.89	8.65	9.15	8.93
NC6	26.73	26.50	25.60	25.69	25.25	CLO	9.69	9.71	9.41	9.76	9.51
NC7	25.16	24.65	24.14	23.98	23.50	D11	-2.10	-1.47	-1.22	0.34	0.50
NC8	23.87	23.45	22.97	22.79	22.23	D12	-6.69	-5.80	-5.31	-3.60	-3.12
NC9	23.07	22.66	22.18	21.98	21.46	MCH	1.72	1.96	1.94	2.82	2.72
C10	22.05	21.74	21.50	21.24	20.69	TCE	-0.82	-0.00	1.03	1.70	2.13
C11	21.87	21.47	21.03	20.66	20.30	CLB	-3.32	-2.84	-2.36	-1.48	-1.25
CC5	25.04	24.97	23.87	24.20	24.24	ACT	19.64	18.96	18.87	18.69	18.22
CC6	24.51	23.98	23.38	23.16	22.76	MEK	11.32	11.25	11.71	11.86	11.57
CC7	21.27	20.78	20.05	19.70	19.34	THF	4.15	4.34	4.61	4.85	4.46
CC8	19.37	18.89	18.33	18.18	17.78	DOX	3.59	4.03	4.66	5.27	5.21
CHX	16.80	16.66	16.18	16.25	16.27	MAC	12.96	13.26	13.85	14.56	14.50
CHD	9.95	10.04	10.03	10.35	10.44	EAC	9.66	10.00	10.49	10.98	11.00
BNZ	0.93	1.36	1.46	2.25	2.49	PAC	7.88	7.99	8.28	8.53	8.43
TOL	1.44	1.85	1.93	2.56	2.96	NBA	6.39	6.61	6.84	7.11	7.03
EBZ	3.48	3.67	3.66	4.14	4.40	EOH	53.83	51.48	49.81	47.84	47.76
CL1	8.85	8.17	6.29	8.31	7.83	POH	32.27	30.66	29.08	27.82	25.82
CL2	-13.94	-12.64	-11.55	-9.21	-8.45	BOH	23.05	21.51	19.96	18.89	17.15
CL3	-19.68	-18.03	-16.33	-13.57	-12.00	AOH	15.20	14.18	13.23	12.62	11.56
CL4	6.57	6.77	7.11	8.09	8.40						

Table 25. Parameters B_{12} for PECH

	$B_{12}/(\text{J}/\text{cm}^3)$						$B_{12}/(\text{J}/\text{cm}^3)$						
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC3	54.66	56.85	43.49	49.92			BCL	17.47	17.35	17.18	16.90	16.52	16.27
NC4	48.55	45.84	43.39	41.80			PCL	16.89	16.76	16.43	15.77	15.68	15.29
NC5	46.25	44.24	41.28	41.15	38.89	39.10	CLH	16.89	16.76	16.42	16.24	15.59	15.30
NC6	40.43	39.33	38.03	37.12	36.35	34.72	CLO	17.97	17.82	17.50	16.93	16.43	16.07
NC7	37.99	36.90	35.74	34.99	33.82	32.73	D11	11.33	11.81	11.64	11.73	11.57	11.39
NC8	36.50	35.46	34.51	33.59	32.66	31.64	D12	5.40	6.42	6.86	7.22	7.57	8.00
NC9	35.45	34.40	33.53	32.53	31.71	30.90	MCH	14.51	13.96	13.72	13.25	13.13	12.72
C10	34.15	33.12	32.32	31.59	30.72	29.87	TCE	16.19	16.72	16.86	16.47	16.43	16.19
C11	33.60	32.66	31.83	30.96	30.05	29.27	CLB	5.88	6.41	6.66	6.69	6.37	6.50
CC5	38.01	36.72	35.75	34.76	34.28	33.20	ACT	11.32	11.87	12.00	10.78	11.77	11.72
CC6	35.80	34.38	33.17	32.41	31.45	30.13	MEK	5.35	6.12	6.59	6.10	6.98	7.02
CC7	31.68	30.39	29.36	28.46	27.43	26.50	THF	-0.86	-0.21	0.08	0.51	0.21	0.39
CC8	28.94	27.88	27.02	26.14	25.20	24.49	DOX	-1.44	-0.23	0.54	0.63	1.62	2.62
CHX	26.29	25.30	24.68	24.28	23.29	22.59	MAC	11.57	12.28	12.85	12.51	13.25	13.92
CHD	18.00	17.38	17.31	16.65	16.59	16.38	EAC	8.64	9.39	9.65	9.74	10.06	10.56
BNZ	7.34	7.06	7.03	7.35	7.12	7.14	PAC	7.37	7.87	8.00	7.96	7.98	8.35
TOL	7.79	7.64	7.73	7.83	7.80	7.99	NBA	6.93	7.43	7.53	7.51	7.56	7.75
EBZ	10.33	10.12	10.05	10.08	9.89	10.01	EOH	82.32	79.27	76.49	72.29	73.37	69.62
CL1	24.40	22.62	17.37	15.46	14.72	14.21	POH	56.32	54.03	51.11	48.21	45.66	43.31
CL2	6.69	7.06	7.00	7.76	8.07	8.06	BOH	44.07	41.88		36.70	34.31	32.69
CL3	5.77	6.36	7.37	8.55	9.36	10.16	AOH	34.23	32.27		28.46	26.68	25.31
CL4	21.65	21.02	20.68	20.22	19.96	19.43							

Table 26. Parameters B_{12} for PHEA

	$B_{12}/(\text{J}/\text{cm}^3)$						$B_{12}/(\text{J}/\text{cm}^3)$						
	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	$t/^\circ\text{C} = 60.0$	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$	
NC7	100.95	100.26	98.18	88.94	82.17	84.52	CHD		77.04	73.14	69.36	69.32	65.93
NC8	98.21	94.40	93.96	90.33	83.79	84.13	BNZ	64.39	58.68	56.15	53.82	53.17	52.92
NC9	91.60	89.96	90.45	86.08	82.20	82.91	TOL	62.06	57.34	56.56	55.00	54.86	54.39
C10	82.30	82.96	85.18	81.89	82.42	81.51	EBZ	61.66	58.67	57.49	56.47	56.17	55.92
C11	75.80	78.42	80.59	79.96	78.35	80.11	CL1	66.07	65.76	56.38	49.23	49.43	46.14
CC5	118.77	120.09	112.18	101.32	102.75	102.73	CL2	40.87	39.25	39.21	38.57	39.57	39.79
CC6	118.98	109.95	103.82	94.75	96.06	89.97	CL3	42.89	40.26	39.99	39.92	41.68	42.70
CC7		103.85	96.96	89.60	87.39	83.33	CL4		80.49	74.99	69.29	67.10	65.09
CC8	102.14	95.65	89.85	85.15	82.26	79.73	BCL	78.68	72.29	69.54	65.62	65.14	63.29
CHX		92.42	86.94	80.85	78.91	76.11	PCL	75.03	69.80	66.72	64.23	63.08	62.12

Table 26 (Continued)

	$B_{12}(\text{J/cm}^3)$						$B_{12}(\text{J/cm}^3)$						
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$		
	60.0	70.0	80.0	90.0	100.0	110.0	60.0	70.0	80.0	90.0	100.0	110.0	
CLH	71.16	67.56	65.14	64.11	63.29	62.34	DOX	24.35	23.13	22.91	22.79	23.53	23.92
CLO	64.74	63.76	63.04	62.86	62.60	62.36	MAC	42.02	40.25	39.82	39.17	39.49	39.07
D11	63.06	56.83	53.69	50.98	50.48	49.12	EAC	44.43	42.41	41.58	40.59	40.74	40.31
D12	42.26	40.67	40.27	39.95	40.55	40.63	PAC	46.02	43.87	42.98	42.10	41.98	41.24
MCH		70.87	65.25	59.98	57.68	55.87	NBA	45.70	44.24	43.54	42.91	42.87	42.35
TCE	64.05	60.97	59.63	58.45	58.83	58.38	EOH	36.80	35.95	35.07	34.56	34.58	35.28
CLB	51.47	50.09	49.58	49.21	49.74	49.61	POH	34.93	33.48	32.64	31.49	31.49	30.70
ACT	34.87	32.38	31.25	30.24	30.02	29.44	BOH	35.33	34.12	32.82	32.00	31.87	31.07
MEK	36.99	35.04	34.25	33.45	33.74	32.98	AOH	33.36	32.72	32.02	31.49	31.66	31.28
THF	36.91	33.79	32.40	31.23	31.92	30.61							

Table 27. Parameters B_{12} for PMA

	$B_{12}(\text{J/cm}^3)$						$B_{12}(\text{J/cm}^3)$						
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$		
	60.0	70.0	80.0	90.0	100.0	110.0	60.0	70.0	80.0	90.0	100.0	110.0	
NC3	65.47	62.31	46.84	43.87			BCL	24.28	22.70	21.66	20.69	20.33	19.99
NC4	60.25	56.38	47.14	43.92			PCL	23.74	22.38	21.38	20.33	19.83	19.26
NC5	61.40	53.10	46.73	45.21	42.66	42.10	CLH	24.02	22.89	22.31	21.47	21.05	20.60
NC6	54.61	48.80	44.88	42.21	40.93	39.77	CLO	25.22	24.42	23.88	23.15	22.65	22.25
NC7	50.40	45.87	42.95	40.65	39.58	38.06	D11	9.08	7.53	7.36	6.82	6.85	7.06
NC8	47.04	43.71	41.49	39.67	38.80	37.51	D12	-0.86	-0.76	-0.05	-0.04	0.69	1.40
NC9	44.51	42.14	40.53	38.93	37.97	36.95	MCH	19.28	15.35	13.84	12.45	11.87	11.54
C10	42.31	40.59	39.53	38.17	37.24	36.02	TCE	14.20	13.56	13.83	13.35	13.38	13.74
C11	41.22	40.05	38.93	37.70	36.77	35.57	CLB	10.38	9.49	8.90	8.63	8.60	9.00
CC5	59.57	51.13	47.15	43.12	41.78	41.43	ACT	17.14	16.43	16.24	15.03	14.77	14.38
CC6	56.49	48.59	44.04	40.91	39.28	38.16	MEK	13.49	13.05	12.96	12.26	12.17	12.17
CC7	48.37	43.17	39.97	37.58	36.20	35.09	THF	13.61	12.72	12.72	11.32	10.97	10.57
CC8	43.13	39.62	37.21	35.48	34.43	33.41	DOX	6.61	6.35	6.52	6.26	6.46	6.98
CHX	41.11	36.75	34.30	32.11	30.94	30.32	MAC	13.02	13.32	13.00	12.56	12.73	12.97
CHD	28.42	25.93	24.56	23.20	22.67	22.54	EAC	12.59	12.30	11.95	11.89	11.95	12.15
BNZ	13.96	12.74	12.10	11.33	11.36	11.41	PAC	13.09	12.56	12.16	11.79	11.66	11.70
TOL	15.57	14.87	14.39	13.79	13.77	13.81	NBA	13.18	12.78	12.41	12.14	11.99	11.98
EBZ	17.38	16.78	16.30	15.69	15.58	15.55	EOH	58.91	54.95	53.02	49.70	47.33	46.22
CL1	17.34	15.21	13.46	11.08	9.95	9.50	POH	39.49	37.69	35.41	32.77	30.62	28.79
CL2	-5.59	-4.97	-4.57	-4.44	-3.64	-2.42	BOH	33.56	30.70	28.40	25.95	24.02	22.43
CL3	-7.26	-6.79	-5.88	-5.29	-3.81	-2.58	AOH	27.57	25.03	22.85	21.03	19.67	18.58
CL4	26.91	23.05	21.17	19.74	19.40	19.23							

Table 28. Parameters B_{12} for PEA

	$B_{12}(\text{J/cm}^3)$					$B_{12}(\text{J/cm}^3)$					
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	
	70.0	80.0	90.0	100.0	110.0	70.0	80.0	90.0	100.0	110.0	
NC3	32.34	25.67	21.46			PCL	12.84	12.49	12.23	12.25	11.34
NC4	33.51	33.05	31.39			CLH		12.95	12.61	12.32	12.14
NC5	31.88	30.25	29.83	28.55	28.75	CLO			13.87	13.74	13.56
NC6	30.07		28.90		27.38	D11	0.39	0.87	0.88	1.38	
NC7	28.91	28.07	27.21	26.51	25.82	D12	-2.87	-2.10	-1.71	-0.67	0.16
NC8	27.95	27.40	26.71	26.21	25.15	MCH	5.36	5.53	5.29	5.32	5.88
NC9	27.41	26.95	26.19	25.83	24.83	TCE	4.86	5.43	5.58	6.08	6.92
C10	26.72	26.12	25.61	25.33	24.35	CLB	2.51	2.92	2.85	3.61	3.98
C11	26.58	25.94	25.31	25.04	24.10	ACT	18.25	18.47		18.91	15.41
CC5	29.12	28.16	27.16	27.34	26.98	MEK	11.94	12.08	12.36	12.18	
CC6	28.46	27.71	26.50	26.11	25.49	THF	6.97	6.64	6.83	6.37	
CC7	26.55	25.93	24.78	24.19	23.26	DOX	7.84	8.15	8.65	8.85	
CC8	24.25	24.49	23.73	23.27	22.53	MAC	13.39	16.57	15.07	13.51	13.66
BNZ	5.51	5.73	5.46	6.00	5.99	EAC	9.90	10.17	10.56	10.06	10.30
TOL	7.34	6.69	7.38	8.00		PAC	8.63	8.71	8.82	8.53	8.49
EBZ	8.76	9.00	8.70	8.82	7.59	NBA	8.02	8.47	8.23	8.10	8.00
CL2	-9.92	-9.09	-8.59	-7.35		EOH	55.80	52.83	49.69	48.92	46.76
CL3	-15.86	-14.32	-13.40	-12.06	-11.18	POH	34.26	33.07	30.33	28.59	26.42
CL4	10.67	10.91	10.80	10.95	10.67	BOH	25.72	24.00	22.19	20.46	18.59
BCL	12.73	12.46	12.00	12.10	11.69						

Table 29. Parameters B_{12} for PBMA

	$B_{12}(\text{J/cm}^3)$					$B_{12}(\text{J/cm}^3)$					
	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	$t/^\circ\text{C} =$	
	70.0	80.0	90.0	100.0	110.0	70.0	80.0	90.0	100.0	110.0	
NC3	19.81	20.08	20.96			NC7	15.79	15.51	14.89	14.72	14.60
NC4	21.72	21.24	20.39			NC8	14.86	14.57	14.00	13.56	13.37
NC5	20.07	21.78	18.63	18.89	19.36	NC9	14.11	13.82	12.92	12.82	12.64
NC6	17.58	17.42	16.34	16.26	16.58	C10	13.20	12.94	12.28	12.17	12.05

Table 29 (Continued)

	$B_{12}/(\text{J}/\text{cm}^3)$						$B_{12}/(\text{J}/\text{cm}^3)$				
	$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$		$t/^\circ\text{C} = 70.0$	$t/^\circ\text{C} = 80.0$	$t/^\circ\text{C} = 90.0$	$t/^\circ\text{C} = 100.0$	$t/^\circ\text{C} = 110.0$
C11	12.96	12.69	11.88	11.75	11.63	D11	2.48	2.99	1.49	2.43	3.92
CC5	18.24	17.62	16.75	16.63	17.58	D12	4.32	4.96	3.62	4.33	6.24
CC6	17.04	16.09	14.72	14.36	14.20	MCH	3.13	2.90	2.76	1.37	2.34
CC7	13.85	13.06	11.61	11.45	11.62	TCE	0.92	1.74	2.17	1.18	2.75
CC8	11.94	11.16	10.34	9.86	9.69	CLB	0.49	0.70	0.96	-0.30	1.08
CHX	12.57	12.08	10.86	10.43	11.02	ACT	32.35	31.95	31.40	29.28	30.09
CHD	9.37	9.10	8.02	7.69	9.29	MEK	18.70	18.72	18.46	17.21	17.60
BNZ	4.97	4.97	4.06	4.99	5.49	THF	8.60	8.58	10.02	7.08	8.09
TOL	4.01	4.14	3.20	4.01	4.62	DOX	16.99	17.41	17.00	15.29	16.28
EBZ	3.80	3.93	4.13	3.66	4.27	MAC	24.83	24.85	24.89	23.33	24.64
CL1	14.86	13.91	13.96	10.20	9.71	EAC	15.95	16.24	16.30	14.92	15.84
CL2	-0.56	0.10	-0.66	0.55	3.20	PAC	11.27	11.49	11.21	9.88	10.64
CL3	-13.14	-11.64	-11.88	-10.99	-8.21	NBA	8.04	8.36	8.22	6.96	7.64
CL4	6.78	6.73	4.96	5.26	6.31	EOH	75.48	73.35	71.59	67.50	66.95
BCL	7.62	7.75	6.13	6.66	7.90	POH	45.80	44.35	42.15	38.23	37.24
PCL	5.75	5.64	3.92	4.06	6.10	BOH	31.93	30.70	28.66	25.03	24.67
CLH	5.38	5.37	5.28	4.04	4.93	AOH	21.36	20.58	19.07	16.33	16.58
CLO	5.28	5.19	5.19	3.90	4.69						

Table 30. Enthalpy of Sorption of Various Probes on Nine Polymers

probe	$-\Delta_{\text{sorp}}H/(\text{kJ mol}^{-1})$										probe	$-\Delta_{\text{sorp}}H/(\text{kJ mol}^{-1})$									
	PEE	PP1	PDMS	PCL	PECH	PHEA	PMA	PEA	PBMA	$\Delta_{\text{vap}}H$		PEE	PP1	PDMS	PCL	PECH	PHEA	PMA	PEA	PBMA	$\Delta_{\text{vap}}H$
NC4	19.66		20.38					18.35	17.70	PCL	33.64	32.93	33.30	35.19	32.76		30.67	32.89		34.56	
NC5	24.64	25.27	24.06						22.89	CLH	38.12	36.40	37.53	38.83	36.48	29.04	34.43	36.74	37.87	38.99	
NC6	29.12	28.83	28.20	25.98	21.71		24.35	26.94	27.91	CLO	46.86	45.48	46.15	46.78	43.76	39.54	41.76	44.52	46.02	48.03	
NC7	33.60		32.34	29.54	25.23		27.24	30.88	32.76	D11	25.31	24.81	25.94	31.25	28.41		28.11	30.12	29.58	27.49	
NC8	37.99	36.86	36.61	33.35	28.95		31.30	34.35	37.45	D12	27.78	27.49	28.45	35.10	33.26	31.00	33.68	34.48	32.97	31.30	
NC9	42.47	38.99	40.79	37.28	32.72		29.08	35.40	38.37	MCH	28.16	26.99	28.53	31.71	28.45		26.19	30.29	29.41	29.08	
C10	46.69		45.90	41.30	36.40		33.18	39.08	42.63	TCE	31.09	29.79	30.92	34.98	31.34	28.37	31.63	33.68	33.43	31.38	
C11	51.00	50.29	48.12	45.15	40.17		36.94	43.10	46.82	51.30	CLB	35.94	33.89	36.11	40.33	38.16	35.15	36.94	39.33	38.16	37.70
CC5	26.74	27.07	26.11	24.85	22.01			23.89	25.36	25.27	ACT	18.87		21.80	28.45	29.37	27.49	27.87		27.03	28.53
CC6	30.38	29.92	29.29	27.32	24.27			25.98	26.69	29.58	MEK	25.48		27.45	32.26	32.89	29.78	30.92		30.38	31.38
CC7	35.52	34.56	34.10	31.92	29.12			30.25	32.13	35.10	THF	27.66	26.78	28.70	30.79	31.34	28.24	28.49	30.21		28.87
CC8	40.29	38.16	38.79	36.48	33.47		29.08	35.98	36.44	40.00	DOX	30.04	28.74	31.71	36.74	31.74	35.48	35.56	36.36	33.60	35.23
CHX	30.63	30.00	29.58	29.58	27.24			28.70	30.12	MAC	23.47		25.69	30.92	30.75	28.24	29.29			28.74	28.53
CHD	29.75	29.12	29.04	30.75	28.87		26.40	29.87	29.79	EAC	27.36		29.54	33.43	33.35	29.33	31.88	32.26	31.34	31.30	
BNZ	28.95	28.37	29.16	32.55	31.13		29.62	31.71	31.59	30.33	PAC	31.71	29.62	33.64	36.69	36.74	31.59	34.77	35.73	34.69	35.65
TOL	33.56	32.13	33.43	36.53	35.02	28.99	33.22	36.19	35.56	34.64	NBA	36.11	34.89	37.78	40.29	40.17	34.85	37.99	39.33	38.41	39.46
EBZ	37.45	35.98	37.23	39.83	38.07	32.26	36.28	37.32	39.20	38.70	EOH			34.22	31.34	38.45	32.68	32.17	31.97	39.66	
CL2	22.76		24.60	31.21	27.91	27.07	28.95	29.91	29.33	25.65	POH	23.60		27.20	37.53	33.68	40.50	35.48	36.32	35.10	43.18
CL3	26.78	24.98	27.74	35.02	30.38	28.45	31.59	33.51	33.01	27.87	BOH	28.28	26.94	31.84	41.25	37.57	43.81	38.70	40.25	39.04	51.84
CL4	29.25	27.53	29.33	31.76	27.70		25.65	29.83		29.25	AOH	32.13	31.25	36.28	45.23	40.92	46.82	41.76		43.10	50.04
BCL	29.12		28.95	31.34	29.16		27.07	29.46		30.00											

Table 31. Three Different Measurements of χ_{12} on PECH Columns at 100 °C

probe	$V_g^a/(\text{cm}^3 \text{g}^{-1})$	χ_{12}^b	χ_{12}^c	χ_{12}^d	probe	$V_g^a/(\text{cm}^3 \text{g}^{-1})$	χ_{12}^b	χ_{12}^c	χ_{12}^d
NC3	0.43	1.869	1.821	1.759	BCL	23.18	0.618	0.616	0.620
NC4	1.10	1.694	1.646	1.735	PCL	43.27	0.645	0.650	0.682
NC5	2.47	1.652	1.628	1.675	CLH	79.06	0.765	0.756	0.761
NC6	4.71	1.717	1.702	1.733	CLO	257.76	0.990	0.984	0.979
NC7	9.10	1.792	1.770	1.779	D11	20.56	0.331	0.334	0.349
NC8	16.47	1.890	1.883	1.887	D12	52.40	0.199	0.209	0.205
NC9	29.79	1.991	1.989	1.994	MCH	24.32	0.455	0.458	0.456
C10	53.66	2.123	2.094	2.102	TCE	37.59	0.528	0.519	0.518
C11	96.26	2.234	2.209	2.218	CLB	162.72	0.242	0.247	0.235
CC5	6.75	1.166	1.124	1.179	ACT	23.29	0.279	0.273	0.275
CC6	13.29	1.252	1.181	1.222	MEK	41.14	0.200	0.201	0.194
CC7	35.61	1.193	1.167	1.176	THF	36.89	0.012	0.017	0.010
CC8	83.75	1.197	1.190	1.183	DOX	102.11	0.043	0.046	0.026
CHX	21.45	0.844	0.835	0.861	MAC	20.20	0.388	0.329	0.359
CHD	28.83	0.562	0.522	0.558	EAC	29.99	0.351	0.354	0.344
BNZ	41.74	0.247	0.229	0.234	PAC	54.03	0.329	0.337	0.323
TOL	79.17	0.307	0.303	0.292	NBA	98.38	0.356	0.338	0.347
EBZ	129.41	0.436	0.438	0.425	EOH	14.16	1.576	1.428	1.485
CL1	3.90	0.369	0.338	0.316	POH	29.70	1.224	1.203	1.194
CL2	18.90	0.182	0.172	0.189	BOH	57.96	1.115	1.123	1.098
CL3	29.09	0.251	0.278	0.273	AOH	110.36	1.029	1.028	1.008
CL4	22.47	0.690	0.682	0.686					

^a V_g values from this work. ^b Previous measurement in the same laboratory on a Perkin-Elmer 3920 GC. ^c Hewlett-Packard 5890 GC, PECH from a different supplier. ^d Varian Aerograph 2100-40 GC, this work.

their extremely short retention volumes (less than 0.4 mL/g).

Although many experimental data have been reported in the area of IGC by several laboratories, the conditions

of the experiments were generally not sufficiently close to each other: we will therefore not compare our data to the literature. In order to get some feeling about the effect of the experimental arrangement on IGC data, we report in Table 31 the χ_{12} values measured by three different researchers in our laboratory, using three different gas chromatographs and two samples of the polymer (PECH) obtained from two different manufacturers. Except for a few probes with a short retention time (propane, butane, methyl chloride—all gases at room temperature with V_g values less than 4 mL/g), and ethanol with a large χ_{12} value, the average differences of χ_{12} are less than 0.01. The reliability of our results can also be determined from the inspection of the data themselves, *i.e.*, from judging the scatter of the χ_{12} values from a presumably smooth dependence on the temperature, or on the number of carbons in a family of related probes interacting with any given polymer or, conversely, for a given probe interacting with a family of similar polymers. Definite correlations are observed. We concluded that our IGC experimental data are reproducible and reliable.

A straightforward thermodynamic calculation links the temperature dependence of V_g to the molar enthalpy of sorption of the probe by the polymer, $\Delta_{\text{sorp}}H$, as

$$d \ln(V_g/T)/d(1/T) = -\Delta_{\text{sorp}}H/R \quad (11)$$

Table 30 lists values of $-\Delta_{\text{sorp}}H$ for nine polymers at six different temperatures. In the last column; the heat of vaporization of the probe at 85 °C is also listed. When calculating $\Delta_{\text{sorp}}H$, we have excluded all V_g values smaller than 10 mL/g. We have also excluded the V_g values obtained on the poly(methyl acrylate) column at 60 °C and on the poly(2-hydroxyethyl acrylate) column at 60 and 70 °C. These measurements were slightly influenced by the slow diffusion of the probes in the polymer phase. While we have estimated that the error caused by the diffusion influences the V_g , χ_{12} , and B_{12} values only to an acceptable degree, we have found that it distorts the V_g vs $1/T$ dependence beyond limits acceptable for calculation of $\Delta_{\text{sorp}}H$.

Equation 11 fitted V_g data quite well. The standard deviation of V_g values was less than 3%, and the absolute error of $\Delta_{\text{sorp}}H$ was less than 0.8 kJ/mol; this compares with the typical value of $\Delta_{\text{sorp}}H$, -25 kJ/mol. It is apparent that for solvents good for a given polymer, $-\Delta_{\text{sorp}}H$ is close to $\Delta_{\text{vap}}H$, while for poor solvents, $-\Delta_{\text{sorp}}H$ is less than $\Delta_{\text{vap}}H$.

It is seen from experimental values listed in the tables that most the solvent-polymer interaction parameters decrease with increasing temperature. Poly(2-hydroxyethyl acrylate) has the largest χ_{12} values for most of our probes, indicating that it has poor interactions with all of our probes (except alcohols). Chloro compounds with slightly acidic character, such as methylene chloride, chloroform, 1,1-dichloroethane, 1,2-dichloroethane, etc., have negative interaction parameters with polycaprolactone, poly(methyl acrylate), and poly(*n*-butyl methacrylate), *i.e.*, with polymers that contain a carboxyl group in the backbone chain or in side groups. This shows strong interaction between acidic moieties and $-\text{COO}$ groups. Aromatic compounds, as well as organic ethers, show

moderately strong interactions with polyepichlorohydrin. We will present a detailed thermodynamic analysis in another paper.

Conclusions

(1) IGC is a quick and reliable method for obtaining the polymer-solvent interaction parameters as well as other thermodynamic properties at the vanishing concentration of solvents. The interaction parameters of 43 common solvents and 9 polymers have been determined in this study. Each polymer-solvent interaction parameter was determined at six different temperatures from 60 to 110 °C.

(2) A number of experimental and analysis refinements were implemented in improving the precision and reproducibility of the thermodynamic data.

(3) Extreme care should be taken in the data treatment when the column temperature nears the critical temperature of a probe; otherwise invalid thermodynamic results will be obtained.

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Received for review November 17, 1993. Accepted July 25, 1994.*

* Abstract published in *Advance ACS Abstracts*, September 1, 1994.