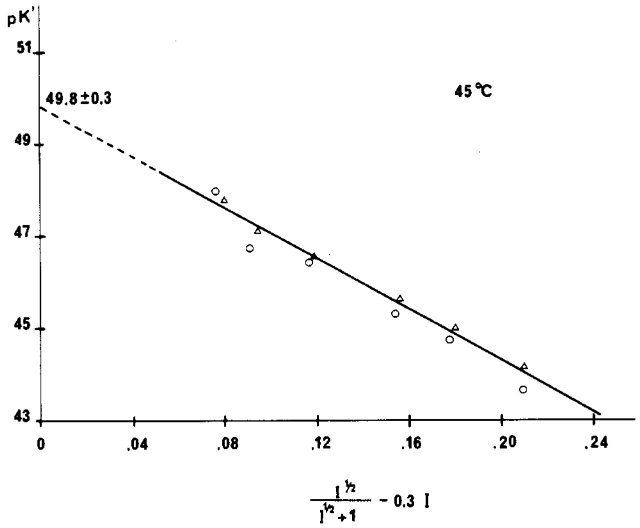

Figure 2. 45 °C plots of pK_{s0} for OCP against $I^{1/2}/(1 + I^{1/2}) - 0.3I$: 12-day equilibration from growth (○) and dissolution (△) experiments.

the calcium and phosphate solutions to the desired pH value of 6.2. This pH was chosen so that after equilibration, the final pH fell in the region 5.5–7.0, in which the exclusive growth of OCP has been demonstrated (*15*). Exploratory measurements made over a range of equilibration times at 25 and 45 °C confirmed that equilibrium at these temperatures required about 14 and 2 days, respectively. The equilibrium data in Table II were obtained after equilibration times of 28 days at 25 °C and 12 days at 45 °C.

The results of the solubility determinations are shown in Tables II and III, and pK'_{s0} values are plotted as a function of ionic strength (eq 3) in Figures 1 and 2. These figures include data obtained from both growth and dissolution experiments and the excellent agreement confirms the attainment of equilibrium. The corresponding values of pK_{s0} obtained by extrapolation to zero ionic strength, 49.6 ± 1.2 and 49.8 ± 0.3 at 25 and 45 °C, respectively, are close to that, 49.3 ± 0.2, obtained at 37 °C (*5*). They confirm the finding that the solubility product of OCP is considerably lower than the value expected from previously reported data (*3*). The mean molar calcium/phosphate ratios of the solid phases after equilibrium in these experiments were 1.30 ± 0.05 at 25 °C and 1.33 ± 0.02 at 45 °C, confirming the good stability of OCP in the aqueous media under these conditions of temperature and pH. In particular, hydrolysis of OCP into an HAP-like phase at 45 °C in the pH range 5.5–6.8 was never detected under the experimental conditions used (see Table III). The marked dependence of solubility of OCP upon ionic strength (see Figures 1 and 2) emphasizes the importance of taking into account activity coefficient corrections when calculating thermodynamic precipitation driving forces in the calcium phosphate systems.

Registry No. $Ca_4H(PO_4)_3$, 13767-12-9.

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Vapor–Liquid Phase Equilibria for the Binaries Isoprene–Dicyclopentadiene and *n*-Pentane–Dicyclopentadiene at 313 and 323 K

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This article presents new total pressure data for the two binary systems, isoprene–dicyclopentadiene and *n*-pentane–dicyclopentadiene, at 313 and 323 K. New vapor pressure data for dicyclopentadiene spanning the temperature range of 313–359 K are also presented. The experimental errors of measurement described as standard deviation are 0.003 mole fraction, 0.03 K, and 0.08 kPa. The data are generally described within the experimental error using a full range vapor pressure equation and a solution model for the total pressures. These are the first data to appear in the literature for these binaries.

Introduction

Three components generally present in isoprene purification are isoprene, *n*-pentane, and dicyclopentadiene (DCPD). Although these C_5–C_{10} binaries are wide boiling and, therefore, easily separated by distillation, it is important to have accurate knowledge of the liquid nonideality for them when studying the ternary isoprene, *n*-pentane, and cyclopentadiene: cyclopentadiene readily dimerizes to DCPD (dicyclopentadiene) at industrially important temperatures. Consequently, any liquid mixture containing cyclopentadiene contains significant amounts of DCPD. Since the literature does not contain phase equilibria data for the isoprene–DCPD and *n*-pentane–DCPD binaries and

Table I. Experimental Dicyclopentadiene Vapor Pressures

T	P_3^0	T	P_3^0	T	P_3^0	T	P_3^0
313.03	1.15	313.08	1.23	323.32	1.55	334.61	2.43
313.05	1.08	313.11	1.03	323.32	1.56	347.56	4.09
313.06	1.16	313.14	1.00	334.59	2.33	359.09	6.53
313.06	1.23	323.31	1.59	334.61	2.47	359.12	6.48

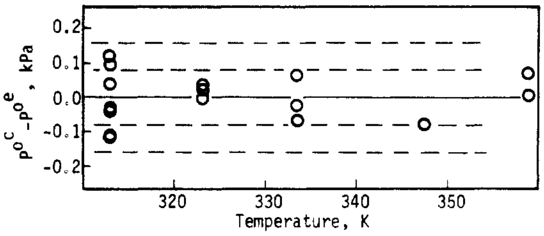

Figure 1. Comparison of calculated pressures from eq 8 to the experimental DCPD vapor pressures.

since there is industrial interest in the fluid-phase behavior of cyclopentadiene and isoprene containing mixtures, we have begun measurements at the Kurata Thermodynamics Laboratory of various C_5 hydrocarbons in combination with DCPD.

This article presents new total pressure data for isoprene and *n*-pentane in combination with DCPD. The temperature range for the study is 313–323 K. In addition, new DCPD vapor pressure data over the temperature range of 313–359 K are presented. A previous article (Howat and Swift (*1*)) presents pure component vapor pressure and total pressure data for the isoprene-*n*-pentane binary from 290 to 330 K.

For the remainder of this article, isoprene is component 1, *n*-pentane is component 2, and DCPD is component 3.

Procedures

The pure component vapor pressures measured for this work and all suitable literature values were fit to the Miller (*2*) equation given as eq 1. The vapor pressures predicted by use

$$\ln (P^0) = A/T + B + CT + DT^2 \qquad (1)$$

of the above equation were used during the determination of solution model coefficients through weighted least squares. The solution model used in this work is that given by Tsuboka and Katayama (*3*) and is repeated below as eq 2–4. The liquid

$$\ln (\gamma_i) = -\ln (\sum_j x_j \Lambda_{ji}) - \sum_k (x_k \Lambda_{ik} / \sum_j x_j \Lambda_{jk}) + \ln (\sum_j x_j \rho_{ji}) + \sum_k (x_k \rho_{ik} / \sum_j x_j \rho_{ik}) \qquad (2)$$

$$\Lambda_{ij} = \rho_{ij} \exp(-(\lambda_{ij} - \lambda_{jj})/RT) \qquad (3)$$

$$\rho_{ij} = v_i / v_j \qquad (4)$$

densities required for the above solution model were calculated by using the correlation of Hankinson and Thomson (*4*) where the characteristic volumes were determined from all suitable literature liquid density data. Vapor-phase fugacity coefficients were calculated by using the Soave–Redlich–Kwong equation of state (Graboski and Daubert (*5*)).

The objective function used in the regression analysis is given as eq 5.

$$S = \sum_j^n (P_j^e - P_j^c)^2 / \sigma^{*2} \qquad (5)$$

$$P^c = \sum_i^2 x_i \gamma_i P_i^0 (\phi_i^0 / \phi_i) \exp(v_i (P_i^0 - P^c)/RT) \qquad (6)$$

$$\sigma^{*2} = \sigma_P{}^2 + (\delta P / \delta x)^2 \sigma_x{}^2 + (\delta P / \delta T)^2 \sigma_T{}^2 \qquad (7)$$

Equation 7 expresses the uncertainty in the total pressure given the uncertainties in pressure, composition, and temperature measurements using propagation of error analysis.

The pure component vapor pressures reported herein are bubble point, static measurements. The mixture total pressure measurements are also static bubble points following the method of Shanker et al. (*6*). Briefly, one component is metered into the test cell. The second component is then incrementally metered into the cell with bubble point measurements being made between increments. The procedure is then repeated with the second component being metered first. By designing the experiments appropriately, the two sets of data overlap at various compositions giving replicated points at each isotherm.

Raw Materials

The isoprene used in this work was donated by Exxon Chemical in Baton Rouge. The pentane used was Phillips Pure Grade. After a 10 theoretical tray distillation column was purged with dry nitrogen, the isoprene and pentane were distilled separately under vacuum at 10 to 1 reflux ratio. The first and last 20% of the charge to the batch column distilled over were discarded. The resultant middle cuts were refrigerated and stored over molecular sieves. The estimated purity of both components was greater than 99.8%. These estimates are based on chromatographic analysis of other samples of isoprene and pentane subjected to the same purification procedures.

DCPD was purchased from the Thiokol Chemical Company with a claimed purity of 98%. Freezing point depression analysis of the raw DCPD indicated that this claim is optimistic with the actual purity varying from bottle to bottle. Purification by distillation was unsuccessful because unstable boiling caused column flooding and freezing DCPD plugged transfer lines. Batchwise, fractional crystallization was finally used to improve the purity. The final purity after repeated crystallization steps was 99.7%. This purity was estimated by using Turnbull and Hull's (*7*) observation that each 0.3 mol % impurity corresponds to 1 K depression of the freezing point from 305.85 K.

Equipment

The cell and manifold assembly used in this work is similar to that used by Shanker et al. (*6*). A mercury manometer was used for pressure reference. An air bath was used for temperature control. Construction details are given in Howat (*8*).

Results

The experimental DCPD data are given in Table I. The 16 points were fit to a truncated Miller equation, eq 8. Figure 1

$$\ln (P_3^0) = 4522/T - 38.95 + 7.862(10^{-2})T \qquad (8)$$

presents a comparison between the experimental data and the above correlation. The root mean square error (RSME) is 0.08 kPa which is consistent with the expected value based on propagation of error. Figure 2 presents a comparison between eq 8 and the literature data which fall in the experimental temperature range. As seen in the figure, the literature DCPD vapor pressure data show significant scatter and the literature vapor pressures are all lower than those of this work. The apparently high experimental vapor pressures could be due to contamination of the sample by light ends which would distort

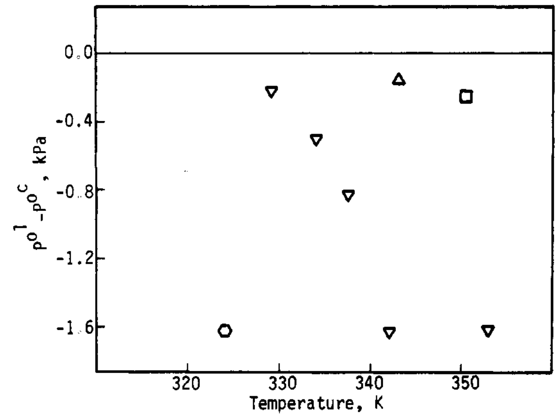

Figure 2. Comparison of literature DCPD vapor pressures to calculated values from eq 8: □, Turnbull and Hull (*7*); △, Stobbe and Reuss (*9*); ○, Ralstrick et al. (*10*); ▽, Wilson and Wells (*11*).

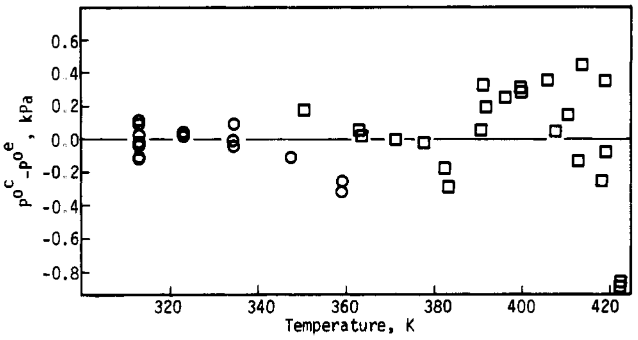

Figure 3. Comparison of calculated DCPD vapor pressures from eq 9 to its data base: ○, this work; □, Turnbull and Hull (*7*).

the bubble point measurement. The DCPD was subjected to 15 min of boiling to remove any residual light components before each vapor pressure measurement. This should have removed these chemicals, thus minimizing the distortion.

The relative uncertainties in the pressure measurement are amplified as the absolute pressure approaches zero. However, the absolute uncertainty remains equivalent to that for higher pressure measurements; i.e., $\sigma^* = 0.08$ kPa. Consequently, random error would not cause the systematic disagreement between the literature and the experimental data.

With the exception of Turnbull and Hull (*7*), none of the references given in Figure 2 provide multiple points. Wilson and Wells (*11*) is a secondary reference reporting prior literature data. No two points attributed to Wilson and Wells come from the same primary reference. The integrity of the data cannot be judged without multiple points.

Vapor pressure coefficients for DCPD were determined by using the data of Table I and the data of Turnbull and Hull (*7*). The resultant equation is

$$\ln (P_3^0) = 14767/T - 138.46 + 3.9940(10^{-1})T - 3.4320(10^{-4})T^2 \quad (9)$$

The above equation describes the data with an RSME of 0.3 kPa. It describes the experimental data of this work to a RSME of 0.1 kPa with a bias of -0.04 kPa. Figure 3 presents the comparison between eq 9 and the data. The difference in description of the data between eq 8 and 9 is statistically significant. However, the predicted pressures are equivalent for the two correlations at 313 and 323 K.

The experimental isoprene and pentane vapor pressures measured by Howat (*8*) have been reported by Howat and Swift (*1*). Table II summarizes the results of the analyses of the vapor pressure data for all three chemicals. Other necessary physical properties for analyzing total pressure data are given in Table III.

Table II. Summary of Pure Component Vapor Pressure Analysis for Isoprene, *n*-Pentane, and Dicyclopentadiene

component	isoprene	*n*-pentane	DCPD
	Experimental Correlation		
no. of points	32	32	16
eq type	Antoine	Antoine	Miller
A	1.37505E+01[a]	1.35539E+01	4.522E+03
B	2.42100E+03	2.33037E+03	-3.895E+01
C	-4.20870E+01	-4.83846E+01	7.862E-02[a]
RSME, kPa	+0.1	+0.1	+0.08
BIAS, kPa	+0.00	+0.00	-0.00
	Overall Correlation		
no. of points	76	99	39
eq type	Miller	Miller	Miller
A	-4.08722E+03	-4.39961E+03	1.4767E+04
B	2.16711E+01	2.45451E+01	-1.3846E+02
C	-1.55520E-02	-2.49796E-02	3.9940E-01
D	1.09142E-05	2.11976E-05	-3.4320E-04
	Description of All Data		
RSME, kPa	+0.1	+0.7	+0.3
BIAS, kPa	+0.00	+0.01	+0.00
	Description of Experimental Data Alone		
RSME, kPa	+0.1	+0.1	+0.1
BIAS, kPa	+0.04	-0.05	-0.04

[a] In this notation, 1.37505E+1 = 1.37505 × 10^1 and 7.8622E-02 = 7.862 × 10^{-2}.

Table III. Pure Component Parameters

component	isoprene	pentane	DCPD
mol wt	68.119	72.151	132.208
critical *T*, K	484	469.6	665
critical *P*, kPa	3850	3374	3060
acentric factor	0.1565	0.2525	0.1837
characteristic vol, m^3/(kg mol)	0.2678	0.3113	0.4113

Table IV. Experimental Isoprene-Dicyclopentadiene Data

Nominal 313.1 K Data

x_1	*T*	*P*	x_1	*T*	*P*
	Set 1			Set 2	
0.049	313.13	9.25	0.900	313.14	111.66
0.100	313.13	16.60	0.797	313.11	99.91
0.149	313.14	23.44	0.707	313.14	89.71
0.199	313.12	30.40	0.605	313.11	78.41
0.299	313.13	43.57	0.499	313.20	66.86
0.499	313.14	67.26	0.399	313.20	55.52
			0.300	313.21	43.84

Nominal 323.1 K Data

x_1	*T*	*P*	x_1	*T*	*P*
	Set 3			Set 4	
0.899	323.15	152.29	0.104	323.11	23.20
0.798	323.13	136.52	0.155	323.14	32.66
0.699	323.15	121.86	0.206	323.13	42.44
0.599	323.15	106.96	0.308	323.14	60.56
0.498	323.16	91.63	0.467	323.10	86.54
0.398	323.19	75.77			
0.299	323.18	59.13			

Table V. Results of Isoprene-Dicyclopentadiene Data Analysis

regression	313.1 K	323.1 K	combined	
no. of points	13	12	25	
$\lambda_{31} - \lambda_{11}$, cal/(g mol)	206	153	180	
$\lambda_{13} - \lambda_{33}$, cal/(g mol)	-5	58	25	
calcd σ^*, %	1.1	0.4	0.9	
expected σ^*, %	1.9	1.2	1.6	
$S/(n-p)$	0.3	0.4	0.4	
regression	313.1 K	323.1 K	313.15 K	323.15 K
γ_1^∞	1.38	1.35	1.38	1.36
γ_2^∞	1.44	1.45	1.45	1.43

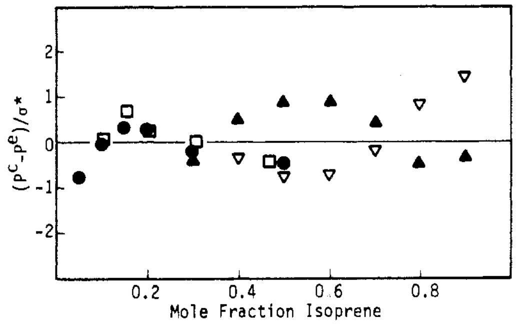

Figure 4. Comparison between calculated and experimental isoprene–DCPD total pressures based on the third regression given in Table V: ●, set 1; ▲, set 2; ▽, set 3; □, set 4.

Table VI. Computed Phase Equilibria for the Isoprene–Dicyclopentadiene Binary

	T = 313.15 K			T = 323.15 K		
x_1	P	y_1	α_{13}	P	y_1	α_{13}
0.0	1.12	0.000	146.0	1.59	0.000	138.2
0.1	16.57	0.938	137.1	22.41	0.935	129.7
0.2	30.66	0.970	128.5	41.53	0.968	121.6
0.3	43.65	0.981	120.2	59.22	0.980	113.7
0.4	55.76	0.987	112.1	75.81	0.986	106.1
0.5	67.21	0.991	104.3	91.58	0.990	98.8
0.6	78.26	0.993	96.8	106.84	0.993	91.8
0.7	89.17	0.995	89.5	121.95	0.995	84.9
0.8	100.18	0.997	82.5	137.26	0.997	78.3
0.9	111.63	0.999	75.6	153.19	0.998	71.9
1.0	123.88	1.000	69.0	170.23	1.000	65.7

The experimental isoprene–DCPD data are listed in Table IV. Three regressions were performed on these data: (1) 313 isotherm alone; (2) 323 isotherm alone; and (3) both isotherms together. The results of these analyses are given in Table V. This table provides the solution model coefficients, calculated uncertainties, expected uncertainty in pressure, and the calculated infinite dilution activity coefficients. The expected error based on propagation of errors is greater than the error in pressure resulting from the regression. Figure 4 presents a scatter diagram showing the deviation between the calculated and experimental pressures: the calculated pressures are based on the third regression given in Table V. All deviations fall within the expected $2\sigma^*$ error bands. This indicates that the solution model does describe the data within the expected error. Another observation is that there is no systematic difference in the residuals of the 313 and 323 isotherms, i.e., the residuals for the 313 data do not fall uniformly above, fall uniformly below, or trend differently with composition from the 323 residuals. This may indicate that the data are internally consistent and that this binary does not exhibit strong temperature dependence over this temperature range. There are no literature data to which these experimental results can be compared. However, a comparison of isoprene or DCPD infinite dilution activity coefficients based on the first two regressions of Table V shows that they are nearly equivalent. The data, therefore, appear internally consistent. Table VI provides the computed phase equilibria for this binary based on the coefficients from the third regression given in Table V.

Table VII. Experimental *n*-Pentane–Dicyclopentadiene Data

Nominal 313.1 K Data

x_2	T	P	x_2	T	P
	Set 1			Set 3	
0.889	313.15	104.11	0.050	313.10	9.76
0.802	313.14	92.99	0.110	313.12	19.72
0.701	313.14	84.74	0.160	313.11	27.09
0.599	313.14	75.43	0.210	313.11	33.97
0.481	313.15	65.17	0.312	313.13	46.92
0.401	313.15	56.96	0.506	313.11	67.14
	Set 2			Set 4	
0.050	313.17	12.08	0.051	313.15	12.56
0.103	313.15	19.11	0.102	313.12	20.25
0.153	313.17	26.68			
0.202	313.17	33.58			
0.301	313.17	46.24			
0.500	313.16	67.22			

Nominal 323.1 K Data

x_2	T	P	x_2	T	P
	Set 5			Set 7	
0.050	323.25	13.60	0.900	323.16	143.93
0.100	323.26	24.74	0.799	323.17	129.94
0.149	323.24	34.62	0.699	323.16	116.91
0.199	323.12	43.88	0.600	323.17	104.44
0.312	323.13	64.25	0.501	323.16	91.27
0.463	323.13	85.59	0.401	323.15	77.50
			0.320	323.14	65.13
	Set 6				
0.897	323.12	142.69		Set 8	
0.800	323.14	129.19	0.053	323.17	13.80
0.699	323.15	116.46	0.103	323.15	24.46
0.600	323.12	103.72	0.152	323.14	34.85
0.482	323.14	88.37	0.203	323.15	44.77
0.400	323.13	76.63	0.254	323.14	53.58
0.300	323.11	61.45	0.396	323.12	76.26

Table VIII. Results of *n*-Pentane–Dicyclopentadiene Data Analysis

regression	313.1 K	323.1 K	combined	
no. of points	20	26	46	
$\lambda_{32} - \lambda_{22}$, cal/(g mol)	259	169	214	
$\lambda_{23} - \lambda_{33}$, cal/(g mol)	129	210	168	
calcd σ^*, %	5.4	1.1	3.9	
expected σ^*, %	2.3	1.8	2.0	
$S/(n-p)$	4.8	0.7	2.6	
regression	313.1 K	323.1 K	313.15 K	323.15 K
γ_2^∞	1.79	1.66	1.73	1.71
γ_3^∞	1.82	1.81	1.83	1.79

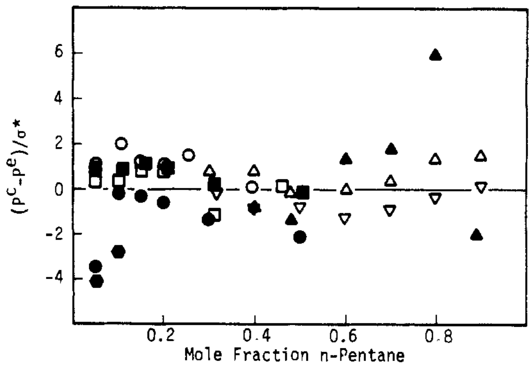

Figure 5. Comparison between calculated and experimental pentane–DCPD total pressures based on the third regression given in Table VIII: ▲, set 1; ●, set 2; ■, set 3; ●, set 4; □, set 5; △, set 6; ▽, set 7; ○, set 8.

The experimental data for the *n*-pentane–DCPD binary are given in Table VII. Table VIII gives the results of three regressions: (1) 313.1 K data alone; (2) 323.1 K data alone; and (3) data of both isotherms together. Comparison of calculated and experimental total pressures based on the third regression of Table VIII is given in Figure 5. The calculated uncertainties in pressure are greater than the expected values for the 313 K isotherm but not for the 323 K isotherm. This is due to greater scatter in the 313 K data. The scatter is shown in Figure 5 but the residuals of the 313 K data are not systematically different from the residuals in the 323 K data.

Table VIII gives predicted infinite dilution activity coefficients based on results of the three regressions. The 313.1 and 323.1 K values for *n*-pentane based on the first two regressions are

Table IX. Computed Phase Equilibria for the *n*-Pentane–Dicyclopentadiene Binary

	T = 313.15 K			T = 323.15 K		
x_2	P	y_2	α_{23}	P	y_2	α_{23}
0.0	1.12	0.000	171.3	1.59	0.000	162.0
0.1	18.52	0.945	153.6	25.00	0.942	145.0
0.2	33.13	0.972	137.4	44.80	0.970	129.7
0.3	45.64	0.981	122.7	61.87	0.980	116.0
0.4	56.64	0.986	109.5	76.99	0.986	103.7
0.5	66.61	0.990	97.5	90.78	0.989	92.4
0.6	75.99	0.992	86.5	103.83	0.992	82.2
0.7	85.19	0.994	76.5	116.67	0.994	72.9
0.8	94.59	0.996	67.4	129.83	0.996	64.4
0.9	104.63	0.998	59.0	143.87	0.998	56.6
1.0	115.80	1.000	51.4	159.45	1.000	49.4

quite different, which is inconsistent with what would be anticipated from the results of the isoprene–DCPD binary. This difference is due to the imprecision in the 313.1 K data. The mixing of pentane and DCPD was particularly difficult at the lower temperature because the DCPD is very viscous at 313 K. Although the isoprene readily mixed with the DCPD despite the viscosity, the pentane–DCPD mixtures required vigorous stirring to mix the pentane layer and the DCPD layer in the cell. The scatter in the experimental data may be due to inadequate mixing. Nevertheless, since the residuals of the two isotherms show the same trends in Figure 5, the data appear to be internally consistent.

Table IX presents the computed phase behavior of the pentane–DCPD binary based on the results of the simultaneous regression of both isotherms.

Conclusions

This article presents new DCPD vapor pressure data and new total pressure data for the isoprene–DCPD and *n*-pentane–DCPD binary pairs. The data are generally described within the experimental errors, although the DCPD vapor pressures near the freezing point are higher than those in the literature. The binary data set for isoprene–DCPD all fall within the expected error bands. Most of the pentane–DCPD data also fall within the error bands, although the data at the lower isotherm show more scatter than the other data presented in this article. There are no data in the literature to which these binary data can be compared.

Glossary

A, B, C, D	Miller coefficients
A, B, C	Antoine coefficients
n	number of measurements
P	pressure (in general), kPa
P^0	vapor pressure, kPa
R	gas constant, cal/(g mol)K
RSME	root mean square error
s	standard deviation, units vary
T	temperature, K
v	component molar volume, m^3/(kg mol)
x	liquid-phase mole fraction
y	vapor-phase mole fraction

Greek Symbols

α	relative volatility, dimensionless
γ	liquid-phase activity coefficient, dimensionless
Λ	solution model interaction parameter, dimensionless
$\lambda_{ij} - \lambda_{jj}$	solution model interaction parameter, cal/(g mol)
ϕ	fugacity coefficient in mixture, dimensionless
ϕ^0	pure component fugacity coefficient, dimensionless
ρ	ratio of molar volumes, dimensionless
σ	standard deviation of measurement, units vary
σ^*	total uncertainty in pressure, kPa

Superscripts

c	calculated value
l	literature value
e	experimental value
∞	infinite dilution

Subscripts

P	pressure
T	temperature
x	composition
1	component 1, isoprene
2	component 2, *n*-pentane
3	component 3, dicyclopentadiene

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Registry No. DCPD, 77-73-6; isoprene, 78-79-5; *n*-pentane, 109-66-0.

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