

# Vapor Pressure, Vapor Density, and Liquid Density for 1,1-Dichloro-1-fluoroethane (R-141b)

Horacio A. Duarte-Garza,<sup>†</sup> Chih-An Hwang, Scott A. Kellerman, Reid C. Miller,<sup>‡</sup> Kenneth R. Hall, and James C. Holste\*

Department of Chemical Engineering, Texas A&M University, College Station, Texas 77843-3122

Kenneth N. Marsh<sup>§</sup> and Bruce E. Gammon

Thermodynamics Research Center, The Texas A&M University System, College Station, Texas 77843-3111

This paper presents measurements of vapor pressures from 250 K to 450 K, liquid densities from 180 K to 370 K at pressures up to 70 MPa, vapor densities at 400 K at pressures up to 1 MPa, and the critical temperature for 1,1-dichloro-1-fluoroethane (R-141b). The derived second and third virial coefficients at 400 K are  $-459.5 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$  and  $1.93 \times 10^{-8} \text{ m}^6 \cdot \text{mol}^{-2}$ . Extrapolating the observed vapor pressures to the measured critical temperature ( $477.5 \pm 0.4$ ) K provides a critical pressure of  $(4.194 \pm 0.002)$  MPa. Using these values with the law of rectilinear diameters indicates a critical density of  $(3921 \pm 6) \text{ mol} \cdot \text{m}^{-3}$ . Correlations provide values which agree with the measured values for liquid densities within  $\pm 0.1\%$  and vapor pressures within  $\pm 0.05\%$ . All uncertainties reported in the paper are  $3\sigma$ .

## Introduction

1,1-Dichloro-1-fluoroethane (R-141b) has been suggested as a possible substitute for trichlorofluoromethane (R-11) in polymer foam blowing applications, but few measurements of its physical properties are available. This paper presents *PVT* values, vapor pressures, vapor densities, and liquid densities (between 180 K and 370 K at pressures to 70 MPa) and the critical temperature.

## Experimental Section

The measurements reported here include vapor pressures, critical temperature, and vapor and liquid densities for R-141b. Summaries of each experimental method appear below; detailed descriptions of these apparatus appear elsewhere.

**Materials.** E. I. du Pont Nemours & Co. provided the sample of R-141b. Their analysis (excluding dissolved air) indicated a sample purity of 99.99+ mol %. Three freeze/thaw cycles removed the dissolved air.

**Vapor Pressure Measurements.** The vapor pressure measurements utilized an isochoric apparatus described by Yurttas (1988). The apparatus consisted of a sample cell surrounded by an isothermal environment. A MINCO platinum resistance thermometer was used to measure the temperature with a precision of  $\pm 0.001$  K and an accuracy of  $\pm 0.01$  K on ITS-90. The pressure was measured with a DH Instruments Model 26000 automatic pressure standard (dead weight gauge) certified accurate to  $\pm 0.005\%$  combined with a differential pressure indicator of our own design which was an integral part of the isochoric cell. The accuracy of the differential pressure indicator was  $\pm 200$  Pa. The samples were loaded into the cell at an overall density slightly higher than the critical density to avoid possible errors caused by adsorption of the sample on the cell wall. Chae *et al.* (1990) noted that R-141b undergoes thermal decomposition above 370 K in the presence of

stainless steel; therefore, a fresh charge of the sample was used for each vapor pressure measurement above this temperature. The exposure time of the samples to the high temperatures did not exceed 2 h. The estimated uncertainty of the vapor pressure measurements is the greater of  $\pm 0.05\%$  or 200 Pa.

**Critical Temperature Measurement.** A cylindrical sapphire cell with an internal volume of about  $4 \text{ cm}^3$  permitted visual determination of the critical point of R-141b by observing the disappearance of the meniscus. The cell was immersed in a well-stirred oil bath where the temperature was measured and controlled within  $\pm 0.01$  K. A Rosemount platinum resistance thermometer, located adjacent to the sample cell, provided the temperature with a precision of  $\pm 0.001$  K and an accuracy of  $\pm 0.01$  K on IPTS-68 (subsequently converted to ITS-90). Because R-141b decomposes at temperatures above 370 K, the experiment restricted the sample exposure time to a maximum of 1.5 h. The estimated uncertainty of the observed critical temperature for R-141b is about  $\pm 0.4$  K.

**Vapor Density Measurement.** A Burnett apparatus, described in detail by Stouffer (1992), provided the vapor densities of R-141b at 400 K. The apparatus consists of two volumes housed in an aluminum enclosure insulated by vacuum and controlled to provide an isothermal environment. The experiment involved expansion of the fluid sample repeatedly from one volume into the second, evacuated volume. Temperature and pressure were measured after each expansion. The densities before and after the expansions were related by the geometry of the apparatus, *i.e.* the ratio of the volume of the first cell to the total volume of both cells. The sequence of expansions during the Burnett experiment produced a series of pressures related by a constant ratio of densities. A nonlinear, statistical analysis of the results, utilizing the virial equation of state, allowed calculation of the densities and virial coefficients without requiring direct measurement of either mass or total volume. The pressure and temperature measurement methods and accuracies were similar to those in the isochoric apparatus. The uncertainties of the derived vapor densities ranged from  $\pm 0.02\%$  at the lowest pressure to  $\pm 0.04\%$  at the highest pressure.

\* Corresponding author.

<sup>†</sup> Current address: Texas A&M University-Kingsville, Kingsville, TX 78363.

<sup>‡</sup> Current address: Washington State University, Pullman, WA 99164.

<sup>§</sup> Current address: University of Canterbury, Private Bag 4800, Christchurch, New Zealand.

**Liquid Density Measurements.** The liquid densities of R-141b were measured with a continuously weighed pycnometer. Lau (1986) described this apparatus in detail. It consisted of a sample cell suspended from an electronic balance surrounded by an isothermal helium bath and copper shield. The mass of sample resulted from weighing, and the volume of the cell came from calibration at several temperatures and pressures with degassed, deionized liquid water. The electronic balance (Arbor Model 507) had a capacity of 0.5 kg and a resolution of  $\pm 0.1$  mg. The sample cell volume was approximately  $10 \text{ cm}^3$ . The pressure of the sample was measured with a strain gauge pressure transducer (Rosemount, Model 1333G10) with an accuracy of  $\pm 0.01$  MPa. A MINCO platinum resistance thermometer (model S-1069) measured the temperature of the sample cell. The thermometer was precise to  $\pm 0.001$  K and accurate to  $\pm 0.01$  K. Although the thermometer was calibrated using IPTS-68, the temperatures reported here have been converted to ITS-90. The estimated uncertainties in the liquid densities are  $\pm 0.1\%$

## Results

The measurements of this work include vapor pressures, compressed liquid densities, superheated vapor densities (along one isotherm), and the critical temperature for R-141b. A description of the various properties follows.

**Vapor Pressures.** The vapor pressure measurements for R-141b, which range from 250 K to 450 K, have been fit to the Iglesias-Silva *et al.* (1987) vapor pressure equation:

$$p(t) = [p_0(t)^N + p_\infty(t)^{1/N}]^{1/N} \quad (1)$$

where

$$p(t) = 1 + (P - P_t)/(P_c - P_t)$$

$$t = (T - T_t)/(T_c - T_t)$$

$$p_0(t) = a_0 + a_1(a_3 t + 1)^{b_0/R} \exp[(-a_2 + b_0/R)/(a_3 t + 1)]$$

$$p_\infty(t) = 2 - a_4(1 - t) + a_5(1 - t)^{2-\theta} + a_6(1 - t)^3 + a_7(1 - t)^4$$

$$a_0 = 1 - P_t/(P_c - P_t)$$

$$a_1 = (1 - a_0) \exp(a_2 - b_0/R)$$

$$a_2 = b_1/RT_t$$

$$a_3 = (T_c - T_t)/T_t$$

$$a_5 = -0.11599104 + 0.29506258a_4^2 - 0.00021222a_4^5$$

$$a_6 = -0.01546028 + 0.0897816a_4^2 - 0.05322199a_4^3$$

$$a_7 = 0.05725757 - 0.06817687a_4 + 0.00047188a_4^5$$

$$N = 87T_t/T_c$$

$$\theta = 0.2$$

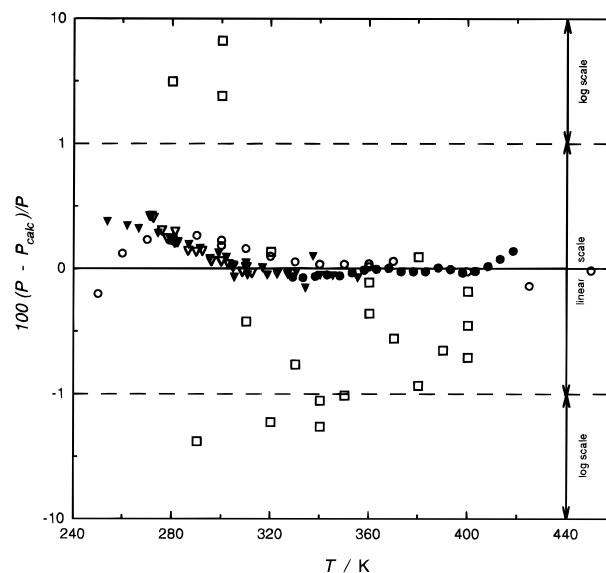
and  $T_t$  is the triple point temperature,  $T_c$  is the critical temperature,  $P_t$  is the triple point pressure, and  $P_c$  is the critical pressure.

**Table 1. Vapor Pressure Measurements for R-141b**

$T/K$	$P/\text{kPa}$	$P_{\text{calc}}/\text{kPa}$	$100(P - P_{\text{calc}})/P$
250.002	8.65	8.67	-0.191
260.000	14.86	14.84	0.130
270.003	24.29	24.24	0.238
279.997	38.06	37.97	0.235
289.995	57.54	57.38	0.270
299.999	84.16	84.00	0.188
300.000	84.20	84.00	0.230
309.999	119.69	119.49	0.164
320.009	165.93	165.77	0.099
330.000	224.76	224.63	0.057
340.000	298.41	298.30	0.036
349.996	389.01	388.87	0.036
359.998	498.93	498.73	0.040
360.002	498.86	498.78	0.016
369.997	630.65	630.27	0.060
399.993	1181.63	1181.90	-0.022
424.996	1859.36	1861.90	-0.136
450.015	2790.89	2791.31	-0.015

**Table 2. Parameters for Equation 1 for the Vapor Pressure of R-141b**

$a_4 = 4.621171$	$P_t = 0.0025 \text{ kPa}$
$b_0 = -54.718127 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$T_c = 477.5 \text{ K}$
$b_1 = 33723.130494 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$P_c = 4194.0 \text{ kPa}$
$T_t = 163.0 \text{ K}$	$R = 8.31448 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$



**Figure 1.** Deviations of the experimental vapor pressures for R-141b from values calculated using eq 1 and the parameters listed in Table 2 (only the vapor pressures measured in this work have been used to determine the parameters). Symbols: (○) this work; (●) Weber (1991); (▽) Weber (1992); (▲) Defibaugh *et al.* (1993); (□) Maezawa *et al.* (1991). The band between  $\pm 1\%$  is a linear scale while those outside  $\pm 1\%$  are log scales, as suggested by Holste *et al.* (1996).

The experimental vapor pressures appear in Table 1. The parameters that provide the best fit of eq 1 are in Table 2. Figure 1 gives the deviations of the experimental and literature vapor pressures from eq 1.

**Critical Temperature.** The critical temperature of R-141b measured by direct observation of the disappearance and reappearance of the vapor-liquid interface was  $(477.5 \pm 0.4) \text{ K}$ . The critical pressure, determined by extrapolating the vapor pressure measurements to the critical temperature, was  $4.194 \text{ MPa}$ . The critical density, determined by extrapolating the saturated vapor and liquid densities to the critical temperature using the law of rectilinear diameters, was  $3921 \text{ mol}\cdot\text{m}^{-3}$ . The saturated vapor densities were calculated using second and third virial coefficients estimated with the Tsonopolous

(1974, 1975) and the Orbey and Vera (1983) correlations, respectively.

**Vapor Densities.** Three Burnett isotherms at 400 K determined the extent of nonideal behavior in the vapor phase. At this temperature, the derived second virial coefficient ( $B$ ) has a value of  $-4.595 \times 10^{-4} \text{ m}^3 \cdot \text{mol}^{-1}$  and the third virial coefficient ( $C$ ) is  $1.93 \times 10^{-8} \text{ m}^6 \cdot \text{mol}^{-2}$ . The Burnett measurements appear in Table 3.

**Liquid Densities.** We have measured liquid densities for R-141b at temperatures between 180 K and 370 K at pressures from slightly above the vapor pressure to about 70 MPa. We have used the 60 measured liquid densities, shown in Table 4, to determine the parameters for a modified Benedict–Webb–Rubin equation of the form

$$\frac{P}{\rho RT} - 1.0 = \sum_{n=1}^8 a_n \rho_r^n + \exp(-\rho_r^2) \sum_{n=9}^{14} a_n \rho_r^{2n-16} \quad (2)$$

where the coefficients are functions of temperature:

$$a_1 = b_1 + b_2 T_r^{-0.5} + b_3 T + b_4 T_r^{-2} + b_5 T_r^{-3}$$

$$a_2 = b_6 + b_7 T_r^{-1} + b_8 T_r^{-2} + b_9 T_r^{-3}$$

$$a_3 = b_{10} + b_{11} T_r^{-1} + b_{12} T_r^{-2}$$

$$a_4 = b_{13} T_r^{-1}$$

$$a_5 = b_{14} T_r^{-2} + b_{15} T_r^{-3}$$

$$a_6 = b_{16} T_r^{-2}$$

$$a_7 = b_{17} T_r^{-2} + b_{18} T_r^{-3}$$

$$a_8 = b_{19} T_r^{-3}$$

$$a_9 = b_{20} T_r^{-3} + b_{21} T_r^{-4}$$

$$a_{10} = b_{22} T_r^{-3} + b_{23} T_r^{-5}$$

$$a_{11} = b_{24} T_r^{-3} + b_{25} T_r^{-5}$$

$$a_{12} = b_{26} T_r^{-3} + b_{27} T_r^{-5}$$

$$a_{13} = b_{28} T_r^{-3} + b_{29} T_r^{-4}$$

$$a_{14} = b_{30} T_r^{-3} + b_{32} T_r^{-4} + b_{32} T_r^{-5}$$

and  $T_r$  is  $T/T_c$ ,  $T_c = 477.5 \text{ K}$ ,  $\rho_r = \rho/\rho_c$ , and  $\rho_c = 3920.9 \text{ mol} \cdot \text{m}^{-3}$ . Equation 2 fits the experimental liquid densities of R-141b within  $\pm 0.1\%$ . Deviations of the experimental liquid densities from eq 2 appear in Figure 2. The parameters of eq 2 for R-141b are in Table 5.

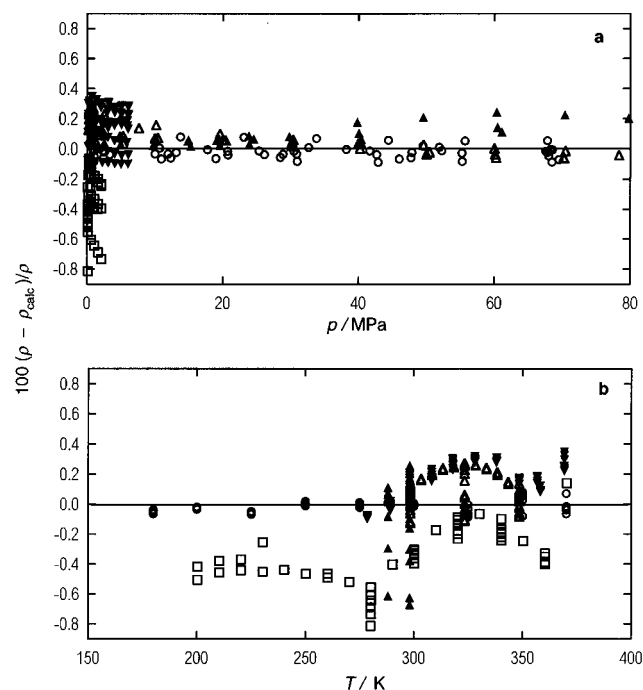
**Smooth Saturation Values.** Smoothed values of the vapor pressure, saturated liquid and vapor densities, enthalpy of vaporization, and entropy of vaporization from 250 K to 370 K appear in Table 6. The enthalpy and entropy of vaporization come from the Clapeyron equation.

## Discussion

**Vapor Pressures.** Weber (1991, 1992) has published vapor pressure measurements for R-141b over most of the range of our measurements. His data include both static and ebulliometric measurements. Defibaugh *et al.* (1993)

**Table 3. Burnett Isotherms for R141b**

$T/\text{K}$	$P/\text{MPa}$	$\rho/\text{mol} \cdot \text{m}^{-3}$	$Z$
Isotherm 1			
400.003	0.975 854	348.37	0.8423
400.001	0.698 612	235.24	0.8930
400.002	0.489 848	158.80	0.9275
400.001	0.339 057	107.20	0.9510
400.001	0.232 803	72.400	0.9668
400.001	0.158 933	48.884	0.9776
Isotherm 2			
399.996	1.045 091	379.30	0.8285
400.001	0.752 540	256.09	0.8836
400.000	0.529 802	172.95	0.9211
400.004	0.367 722	116.80	0.9466
400.000	0.252 788	78.856	0.9639
400.000	0.172 722	53.233	0.9756
400.002	0.117 592	35.950	0.9835
Isotherm 3			
399.999	0.905 355	318.10	0.8558
400.007	0.644 767	214.89	0.9021
400.006	0.450 565	145.09	0.9337
399.998	0.311 376	98.022	0.9551
399.998	0.213 397	66.171	0.9697
400.003	0.145 530	44.673	0.9795



**Figure 2.** Deviations of the measured compressed liquid densities for R-141b from values calculated from eq 2 and the parameters listed in Table 5. Only the liquid densities measured in this work are used to determine the parameters of eq 2. Symbols: (○) this work; (▼) Defibaugh *et al.* (1993); (□) Maezawa *et al.* (1991); (△) Matsuo *et al.* (1994); (▲) Malhotra and Woolf (1994). Figure 2a has pressure for the  $x$ -axis, while (b) has temperature for the  $x$ -axis.

report ebulliometric vapor pressure measurements from 254 K to 356 K. Maezawa *et al.* (1991) also have reported static vapor pressure measurements for R-141b from 200 K to 400 K for which the estimated accuracy of pressure measurement is  $\pm 10 \text{ kPa}$ . Figure 1 compares the results of Weber, Defibaugh *et al.*, and Maezawa *et al.* with the present work. The agreement with Weber and Defibaugh *et al.* is within the combined error estimates of the laboratories, and the differences exceed  $\pm 0.1\%$  only at lower temperatures where the vapor pressures are below atmospheric pressure and the accuracy and precision of our measurements are limited by the  $\pm 200 \text{ Pa}$  accuracy of the difference pressure indicator. The Maezawa *et al.* results

**Table 4. Pycnometric Measurements of Liquid Densities for R-141b<sup>a</sup>**

<i>T</i> /K	<i>P</i> /MPa	$\rho$ /mol·m <sup>-3</sup>	$\rho_{\text{cal}}$ /mol·m <sup>-3</sup>	% dev
180.000	67.9626	12 814.8	12 820.7	-0.046
180.000	46.0230	12 692.7	12 701.0	-0.066
180.000	26.0793	12 578.1	12 582.8	-0.037
180.000	2.4220	12 417.9	12 425.4	-0.060
200.000	67.8427	12 555.6	12 558.5	-0.023
200.000	47.8593	12 432.9	12 435.8	-0.023
200.000	28.8572	12 304.1	12 308.5	-0.035
200.000	11.9112	12 178.8	12 182.9	-0.033
200.000	2.5178	12 104.6	12 106.9	-0.019
225.000	69.4701	12 258.0	12 266.6	-0.070
225.000	47.7627	12 106.5	12 113.6	-0.058
225.000	28.4667	11 956.6	11 963.4	-0.057
225.000	12.3052	11 816.3	11 823.4	-0.060
225.000	1.0389	11 709.5	11 715.4	-0.050
250.000	68.4842	11 965.1	11 965.7	-0.005
250.000	49.5336	11 816.9	11 814.8	0.017
250.000	32.6178	11 668.0	11 667.1	0.007
250.000	17.6870	11 521.7	11 522.5	-0.007
250.000	2.3675	11 352.2	11 353.8	-0.014
275.000	68.1572	11 669.7	11 670.3	-0.005
275.000	51.9272	11 527.6	11 526.4	0.010
275.000	38.1943	11 393.2	11 393.6	-0.003
275.000	25.2904	11 254.4	11 256.1	-0.015
275.000	13.1431	11 108.3	11 111.0	-0.024
275.000	1.8141	10 955.5	10 955.6	-0.001
300.000	68.2394	11 378.6	11 379.4	-0.007
300.000	52.2806	11 220.1	11 221.4	-0.012
300.000	41.6613	11 104.7	11 106.3	-0.014
300.000	30.4320	10 970.7	10 972.6	-0.017
300.000	20.6606	10 841.1	10 842.9	-0.017
300.000	10.6851	10 693.3	10 692.9	0.004
300.000	0.9160	10 519.2	10 520.8	-0.015
325.000	68.4504	11 084.3	11 093.8	-0.085
325.000	55.2897	10 940.9	10 949.9	-0.082
325.000	42.9194	10 790.2	10 799.8	-0.089
325.000	30.9516	10 627.0	10 635.8	-0.083
325.000	18.9233	10 438.0	10 444.8	-0.065
325.000	10.0334	10 276.4	10 279.9	-0.034
325.000	1.0110	10 083.7	10 084.0	-0.003
350.000	67.8037	10 813.3	10 807.5	0.054
350.000	55.7010	10 665.8	10 660.2	0.052
350.000	44.3954	10 512.5	10 506.6	0.057
350.000	33.7802	10 350.5	10 343.5	0.068
350.000	23.0588	10 161.9	10 154.1	0.077
350.000	13.7585	9 971.1	9 963.3	0.078
350.000	5.4285	9 767.3	9 764.8	0.026
350.000	0.9636	9 636.6	9 644.6	-0.083
370.000	67.5313	10 589.6	10 591.3	-0.016
370.000	55.2705	10 426.5	10 429.5	-0.028
370.000	42.6803	10 236.0	10 239.9	-0.038
370.000	30.8477	10 028.5	10 031.9	-0.034
370.000	20.7155	9 817.5	9 821.5	-0.041
370.000	10.9475	9 569.6	9 575.9	-0.066
370.000	3.3592	9 326.3	9 329.9	-0.038
370.000	1.0218	9 237.6	9 231.2	0.070

<sup>a</sup> A molecular weight of 116.9505 was used to convert the measured mass densities to the molar densities given in this table.

are generally within  $\pm 1.0\%$ , but the maximum deviation is 13.4%.

**Vapor Densities.** Weber (1991) has reported vapor density measurements for R-141b measured using a Burnett-isochoric technique. His Burnett isotherm is 393.17 K, while our value is 400.0 K. This precludes convenient direct comparisons, but our result for the second virial coefficient of  $-459.5 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$  is qualitatively consistent with his value of  $-483.7 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$ . Goodwin and Moldover (1991) derived second virial coefficients from their sound speed measurements from 260.00 to 393.15 K. Their extrapolated value at 400 K is  $-459.2 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$ , in excellent agreement with the current value. The Tsionopolous correlation predicts a value for the

**Table 5. Parameters for Equation 2 for the Liquid Density of R-141b<sup>a</sup>**

$b_1 = -12.813\ 627$	$b_{22} = -401.004\ 781$
$b_8 = 10.088\ 032$	$b_{25} = 51.864\ 086$
$b_{10} = 2.533\ 089$	$b_{27} = -9.624\ 144$
$b_{13} = -0.842\ 929$	$b_{28} = 2.484\ 318$
$b_{15} = -0.678\ 084$	$b_{29} = -0.104\ 951$
$b_{17} = -0.005\ 159$	$b_{30} = -0.556\ 224$
$b_{18} = 0.128\ 610$	$b_{31} = 0.230\ 983$
$b_{19} = -0.021\ 879$	$b_{32} = 0.025\ 244$
$b_{20} = 1908.906\ 627$	$T_c = 477.5\ \text{K}$
$b_{21} = -891.124\ 773$	$\rho_c = 3920.9\ \text{mol} \cdot \text{m}^{-3}$

<sup>a</sup> All  $b_i$  values not listed explicitly are equal to zero.

**Table 6. Smoothed Values of Properties along the Saturation Line for R-141b**

<i>T</i> /K	$P_{\text{sat}}$ /kPa	$\rho_{\text{vap}}$ /mol·m <sup>-3</sup>	$\rho_{\text{liq}}$ /mol·m <sup>-3</sup>	$\Delta_{\text{vap}}H$ /J·mol <sup>-1</sup>	$\Delta_{\text{vap}}S$ /J·mol <sup>-1</sup> ·K <sup>-1</sup>
250.000	8.676	4.2056	11 325.4	2892.7	11.571
255.000	11.414	5.4328	11 247.9	2870.7	11.258
260.000	14.835	6.9377	11 169.6	2848.7	10.957
265.000	19.063	8.7646	11 090.3	2825.4	10.662
270.000	24.234	10.9612	11 010.1	2800.9	10.374
275.000	30.497	13.5787	10 928.7	2775.8	10.094
280.000	38.012	16.6714	10 846.1	2749.7	9.820
285.000	46.953	20.2978	10 762.3	2722.6	9.553
290.000	57.503	24.5187	10 677.4	2694.8	9.292
295.000	69.855	29.3979	10 591.4	2666.1	9.038
300.000	84.215	35.0038	10 504.5	2636.7	8.789
305.000	100.796	41.4070	10 416.9	2606.6	8.546
310.000	119.820	48.6817	10 328.8	2575.8	8.309
315.000	141.516	56.9053	10 240.5	2544.5	8.078
320.000	166.123	66.1602	10 152.3	2512.5	7.852
325.000	193.886	76.5327	10 064.5	2480.0	7.631
330.000	225.057	88.1139	9 977.1	2447.0	7.415
335.000	259.895	101.0009	9 890.1	2413.6	7.205
340.000	298.666	115.2971	9 803.4	2379.7	6.999
345.000	341.644	131.1139	9 716.3	2345.3	6.798
350.000	389.112	148.5722	9 628.2	2310.5	6.601
355.000	441.360	167.8034	9 537.6	2275.2	6.409
360.000	498.687	188.9507	9 442.3	2239.4	6.221
365.000	561.404	212.1732	9 337.6	2203.0	6.036
370.000	629.832	237.6476	9 212.4	2165.7	5.853

**Table 7. Critical Constants and Acentric Factor for R-141b**

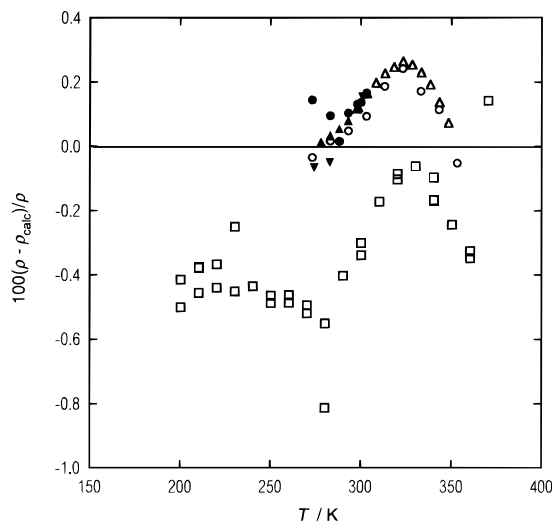
	$T_c$ /K	$P_c$ /kPa	$\rho_c$ /mol·m <sup>-3</sup>	$Z_c$	$\omega$
this work	477.5 $\pm 0.4$	4194.0 $\pm 2$	3920.9 $\pm 6$	(0.2694 $\pm$ 5) $\times 10^{-4}$	0.2178
Chae <i>et al.</i> (1990)	477.3	4229.0 <sup>a</sup>	3941.8	0.2703	0.2237 <sup>a</sup>

<sup>a</sup> From vapor pressure data by Defibaugh *et al.* (1993).

second virial coefficient of  $-512 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$  at 393.17 K and of  $-491 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$  at 400 K. The deviation of our  $B$  value from the predicted value is +6.7%, while the Weber  $B$  deviates from the predicted value by +5.5%. The difference of  $5 \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$  is within the combined uncertainty of the two sets of measurements.

**Critical Temperature.** Chae *et al.* (1990) report an indirect determination of the critical temperature and density for a number of hydrofluorocarbons and hydrochlorofluorocarbons, including R-141b, from analysis of refractive index measurements up to about 1 K below the critical temperature. They report a value of 477.3 K for the critical temperature and a value of 3941.8 mol·m<sup>-3</sup> for the critical density. Our values agree with these values within the estimated experimental uncertainty. A summary of critical and reducing parameters for R-141b appears in Table 7.

**Liquid Densities.** Defibaugh *et al.* (1993) report liquid density measurements for R-141b at temperatures from



**Figure 3.** Deviations of measured saturated liquid densities from values extrapolated from eq 2. Symbols: (▼) Defibaugh *et al.* (1993); (○) Kumagai and Takashi (1993); (□) Maezawa *et al.* (1991); (▲) Malhotra and Woolf (1994); (△) Matsuo *et al.* (1994); (●) Sousa *et al.* (1994).

278 K to 370 K with pressures up to 6.0 MPa. Maezawa *et al.* (1991) have published liquid densities for R-141b from 200 K to 400 K with pressures up to 2 MPa. Parts a and b of Figure 2 compare these results with the present work. The values reported by Defibaugh *et al.* are from 0.1% to 0.35% higher than our values. The liquid densities reported by Maezawa *et al.* are from 0.2% to 0.7% lower than our values. Matsuo *et al.* (1994) report values which agree with this work within  $\pm 0.28\%$ . Malhotra and Woolf (1994) provide ratios of liquid densities; the isotherms for which they provide the reference density agree with the present work within  $\pm 0.02\%$  in the region of overlap. In addition, saturated liquid densities are available from Defibaugh *et al.* (1993), Kumagai and Takashi (1993), Maezawa *et al.* (1991), Malhotra and Woolf (1994), Matsuo *et al.* (1994), and Sousa *et al.* (1994). Figure 3 presents the deviations of these data from the saturated liquid densities extracted from eq 2. All the data are within  $\pm 0.2\%$  of eq 2 except those of Maezawa *et al.* which are mostly within  $-0.5\%$ .

## Conclusions

This paper presents accurate measurements of vapor pressures, compressed liquid densities, superheated vapor densities, and critical temperatures for R-141b. Our measurements span a wide range of temperature (180 K to 477.5 K) and pressure (0.1 MPa to 70.0 MPa). The accuracy of the vapor pressures is the greater of  $\pm 0.05\%$  or 200 Pa. Agreement with other reported measurements is within the combined error estimates. The liquid densities have accuracies of  $\pm 0.1\%$ . Our liquid density values are lower than those reported by Defibaugh *et al.* (1993) (from 0.1% to 0.35%) and higher than those reported by Maezawa *et al.* (1991) (from 0.2% to 0.7%) but agree quite well with those of Malhotra and Woolf (1994) and Matsuo *et al.* (1994). Our critical temperature measurement agrees with the value derived by Chae *et al.* (1990) within the estimated experimental uncertainty. For the vapor density measurements, we have no direct comparison with other reported values. The value for our second virial coefficient

at 400 K is in excellent agreement with the value extrapolated from the second virial coefficients derived from the speed of sound measurements by Goodwin and Moldover (1991).

## Acknowledgment

The authors acknowledge gratefully E. I. du Pont Nemours & Co. for providing the sample used in this work.

## Literature Cited

- Chae, H. B.; Schmidt, J. W.; Moldover, M. R. Alternative refrigerants R123a, R134, R141b, R142b, and R152a: critical temperature, refractive index, surface tension, and estimates of liquid, vapor, and critical densities. *J. Phys. Chem.* **1990**, *88*, 8840–8845.
- Defibaugh, D. R.; Goodwin, A. R. H.; Morrison G.; Weber L. A. Thermodynamic properties of 1,1-dichloro-1-fluoroethane (R141b). *Fluid Phase Equilib.* **1993**, *85*, 271–284.
- Goodwin, A. R. H.; Moldover, M. R. Thermophysical properties of gaseous refrigerants from speed-of-sound measurements. II. Results for 1,1-dichloro-1-fluoroethane (CCl<sub>2</sub>FCH<sub>3</sub>) *J. Chem. Phys.* **1991**, *95*, 5230–5235.
- Holste, J. C.; Hall, K. R.; Iglesias-Silva, G. A. Log-linear plots for data representation. *AIChE J.* **1996**, *296*–297.
- Iglesias-Silva, G. A.; Holste, J. C.; Eubank, P. T.; Marsh, K. N.; Hall, K. R. A vapor pressure equation from extended asymptotic behavior. *AIChE J.* **1987**, *33*, 1550–1556.
- Kumagai, A.; Takashi, S. Saturated liquid viscosities and densities of environmentally acceptable hydrochlorofluorocarbons (HCFCs). *Int. J. Thermophys.* **1993**, *14*, 339–342.
- Lau R. A continuously weighed pycnometer providing densities for carbon dioxide + ethane mixtures between 240 and 350 K at pressures up to 35 MPa. Ph.D. Dissertation. Texas A&M University, College Station, TX, 1986.
- Maezawa Y.; Sato H.; Watanabe, K. Liquid densities and vapor pressures of 1,1,2,2-tetrafluoroethane (HFC 134) and 1,1-dichloro-1-fluoroethane (HCFC 141b). *J. Chem. Eng. Data* **1991**, *36*, 151–55.
- Malhotra, R.; Woolf, L. A. Volumetric measurements for 1,1-dichloro-1-fluoroethane (R141b) in the temperature range 278.15 to 338.15 K and pressure range from 0.1 to 380 MPa. *Fluid Phase Equilib.* **1994**, *92*, 195–213.
- Matsuo, S.; Tanaka, Y.; Kubota, H.; Makita, T. Liquid Densities of HCFC 225ca, HCFC 225cb, and HCFC 141b *J. Chem. Eng. Data* **1994**, *39*, 903–906.
- Orbey, H.; Vera, J. H. Correlation for the third virial coefficient using  $T_c$ ,  $p_c$  and  $\omega$  as parameters. *AIChE J.* **1983**, *29*, 107–113.
- Sousa, A. T.; Fialho, P. S.; Nieto de Castro, C. A. The density of 1,1-dichloro-1-fluoroethane (HCFC 141b). *Int. J. Thermophys.* **1994**, *15*, 375–377.
- Stouffer, C. E. Densities of mixtures of carbon dioxide and hydrogen sulfide from 200 to 450 K to 23 MPa by the Burnett-isochoric method. Ph.D. Dissertation. Texas A&M University, College Station, TX, 1992.
- Tsonopoulos, C. An empirical correlation of second virial coefficients. *AIChE J.* **1974**, *20*, 263–272.
- Tsonopoulos, C. Second virial coefficients of polar haloalkanes. *AIChE J.* **1975**, *21*, 827–829.
- Weber, L. A. PVT and thermodynamic properties of R141b in the gas phase. Proceedings of the XVIIIth International Congress of Refrigeration, Montreal, Canada, August 10–17, 1991.
- Weber, L. A. Ebuliometric measurement of the vapor pressures of R123 and R141b. *Fluid Phase Equilib.* **1992**, *80*, 141–148.
- Yurttas, L. A new isochoric apparatus with applications to P-V-T measurements and phase equilibria studies. Ph.D. Dissertation. Texas A&M University, College Station, TX, 1988.

Received for review November 14, 1996. Accepted January 16, 1997. The majority of the funding for this work has been provided by the American Society of Heating, Refrigerating, and Air Conditioning Engineers. Additional support has come from the Governor's Energy Management Center—State of Texas Energy Research in Applications (Contract No. 5217), the Center for Energy and Mineral Resources at Texas A&M University, and the Texas Engineering Experiment Station.

JE9603584

Abstract published in *Advance ACS Abstracts*, March 1, 1997.