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Vapor Pressure and Gas Phase *P*−*V*−*T* Data for 1,1,1,3,3-Pentafluoropropane (R-245fa)

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A constant-volume apparatus was used to measure the vapor pressure and single phase properties (*P*−*V*−*T*) for 1,1,1,3,3-pentafluoropropane (R-245fa), an ozone-friendly refrigerant. The measurements were done from 265 K to 367 K and at pressures from 35 kPa to 610 kPa. The 51 experimental points taken for the vapor pressure region were fitted with the Antoine equation. The 32 experimental *P*−*V*−*T* measurements in the superheated vapor region taken along four isochores were regressed to the virial equation of state in the Leiden form truncated after the second term. Consistency of the derived second virial coefficients was shown with the Tsonopoulos and Weber correlating methods. The experimental results were also compared with the few data available in the literature.

Introduction

1,1,1,3,3-Pentafluoropropane (R-245fa) has zero ozone depletion potential and a low global warming potential. For these reasons, this refrigerant is currently considered to be a promising replacement for chlorine-containing compounds such as 1,1-dichloro-1-fluoroethane (R-141b) and 1,2-dichloro-1,1,2,2-tetrafluoroethane (R-114) in high-temperature heat pumps and chemical blowing agents.

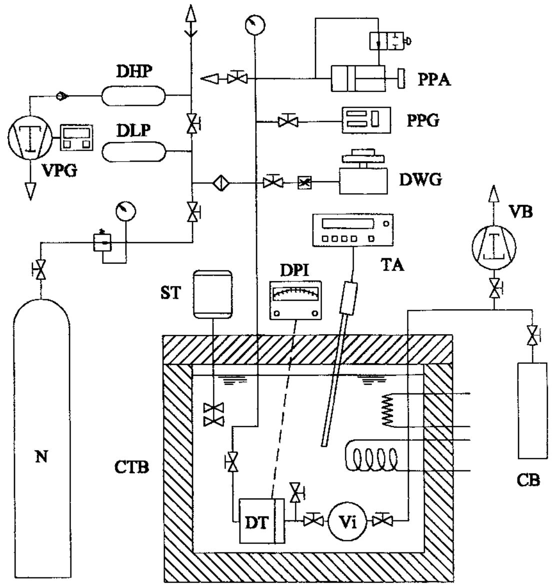
Its physical properties have recently been the object of study.[1,2] Several publications have also dealt with viscosity,[3] static dielectric constant,[4] and compressed and saturated liquid densities.[5] The vapor pressures for R-245fa have been measured over a wide range of temperatures by means of a constant-volume apparatus[6] and at a few points using a VLE apparatus.[7−9] To our knowledge, the only available data in the superheated vapor region have been reported in ref 6.

To partially fill the gaps and to continue the extensive research work that has been carried out by our laboratories on the thermophysical properties of the propane derivatives[10,11] and their mixtures,[12,13] measurements on vapor pressures and in the superheated region on R-245fa have been performed.

Experimental Section

Materials. The sample was provided by Allied Signal. It was deaereated by immersion in liquid nitrogen and evacuation. Its purity was checked by gas chromatographic analysis and was found to be >99.97%, based on area response by using a thermal conductivity detector.

Apparatus. The experimental apparatus is schematically illustrated in Figure 1. A classical constant-volume apparatus with a volume of ∼254 cm^3 was used. The apparatus has been described in detail elsewhere.[14,15] A stainless steel spherical cell contains the refrigerant sample and is connected to a differential diaphragm pressure transducer, coupled to an electronic null indicator. The spherical cell and pressure transducer are immersed in the main thermostatic bath containing a mixture of water and glycol and controlled by a proportional integrative derivative (PID) device. An auxiliary bath, also controlled by a PID device, helps the system to keep the temperature constant. A platinum resistance thermometer is immersed near the cell and is connected to a digital indicator. The instrument is calibrated on the ITS-90, and its uncertainty is certified as being within ±15 mK. The pressure measurement is obtained with a dead weight guage with an experimental uncertainty in the pressure measurements of ±0.5 kPa.



Nomenclature:

CB	Charging Bottle	PPA	Precision pressure controller (Ruska, mod. 3891)
CTB	Main thermostatic bath	PPG	Vibr. cylinder pressure gage (Ruska, mod. 6220)
DHP	High pressure expansion chamber	ST	Stirrer
DLP	Low pressure expansion chamber	TA	Platinum resistance Thermometer (Delta, PT100)
DPI	Electronic null indicator (Ruska, mod. 2461)	VB	Vacuum pump (Vacuubrand , mod. RZ2)
DT	Differential prresure transducer (Ruska, mod. 2413)	Vi	Constant volume spherical cell
DWG	Gas lubricated dead weight gage (Ruska, mod 2465)	VPG	Vacuum pump gage (Galileo, mod. OG510)
N	Nitrogen reservoir		

Figure 1. Schematic drawing of the apparatus.

The charging procedure for a one-component system is as described elsewhere.[10] The uncertainty in the measurement of the mass inside the cell is estimated in the same

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Table 1. Experimental Saturation Pressures for R-245fa

T_{90}/K	P/kPa	T_{90}/K	P/kPa	T_{90}/K	P/kPa
264.69	35.3	297.41	144.1	317.95	292.2
267.89	41.3	297.97	147.1	319.93	311.1
269.95	45.6	299.61	156.2	321.89	330.5
271.90	49.9	299.96	158.2	323.92	351.6
273.96	54.9	301.60	168.0	325.88	373.1
275.92	59.9	301.95	170.1	327.87	396.0
277.98	65.7	303.50	179.8	329.98	421.2
279.99	71.7	303.99	182.9	331.84	444.4
281.99	78.1	305.43	192.4	333.48	465.9
283.89	84.6	305.99	196.2	335.84	497.9
285.94	92.1	308.44	213.5	337.65	523.8
287.94	99.9	309.50	221.5	341.84	586.7
290.01	108.4	311.01	232.9	343.85	619.2
291.63	115.5	313.51	253.0	345.75	650.7
292.01	117.4	313.91	256.6	347.75	685.5
293.40	123.7	315.57	270.6	349.50	717.1
296.05	136.9	315.95	274.2	351.88	761.5

way, amounting to ±10 mg for this sample. The volume of the cell, piping, and pressure transducer cavity is measured with an uncertainty of ± 0.0003 dm^3. From the uncertainties in the mass and volume measurements, the uncertainty in calculated molar volume was estimated to be always lower than ± 0.07 dm^3·mol^{-1}.

The overall experimental uncertainty in terms of pressure, calculated using the laws of error propagation, was estimated to be lower than ±0.7 kPa for measurements along the saturation line and lower than ±1.2 kPa in the superheated vapor region.

Results and Discussion

Vapor Pressure. The experimental vapor pressures in a temperature range from 265 K to 352 K are given in Table 1. Experimental data were fitted with one of the most popular equations, the three-parameter Antoine equation:

$$\log P = A - B/(C + T) \tag{1}$$

The following values were found for the parameters: $A = 14.235437$, $B = 2303.742$, and $C = -48.765$, with d$P = -0.01\%$ and abs(dP) $= 0.03\%$.

Deviations in pressure are defined as

$$\mathrm{d}P = \frac{1}{n}\sum_{i=1}^{n}[(P_{\mathrm{exptl}} - P_{\mathrm{calcd}})/P_{\mathrm{exptl}} \times 100] \tag{2}$$

$$\mathrm{abs}(\mathrm{d}P) = \frac{1}{n}\sum_{i=1}^{n}[\mathrm{abs}(P_{\mathrm{exptl}} - P_{\mathrm{calcd}})/P_{\mathrm{exptl}} \times 100] \tag{3}$$

where n is the number of experimental points. The error distribution is shown in Figure 2.

Our experimental results were also compared with published data. Apart from a few points measured with an uncertainty lower than ±1 kPa by means of a direct method,[7−9] to our knowledge only ref 6 reports a wide range of vapor pressures for this compound. In ref 6, the authors reported vapor pressure measurements with two different experimental apparatus, one for temperatures up to 343 K and a second for temperatures from 343 K to near the critical point. The overall uncertainty in the vapor pressure was estimated to be less than ±5 kPa by these authors. Comparison of the literature data with the Antoine equation (eq 1) shows good agreement with refs 7−9, whereas a poor agreement was found with ref 6; however, it was within the experimental uncertainty. The error distribution, together with deviations calculated using REFPROP 6.0,[16] is shown in Figure 3.

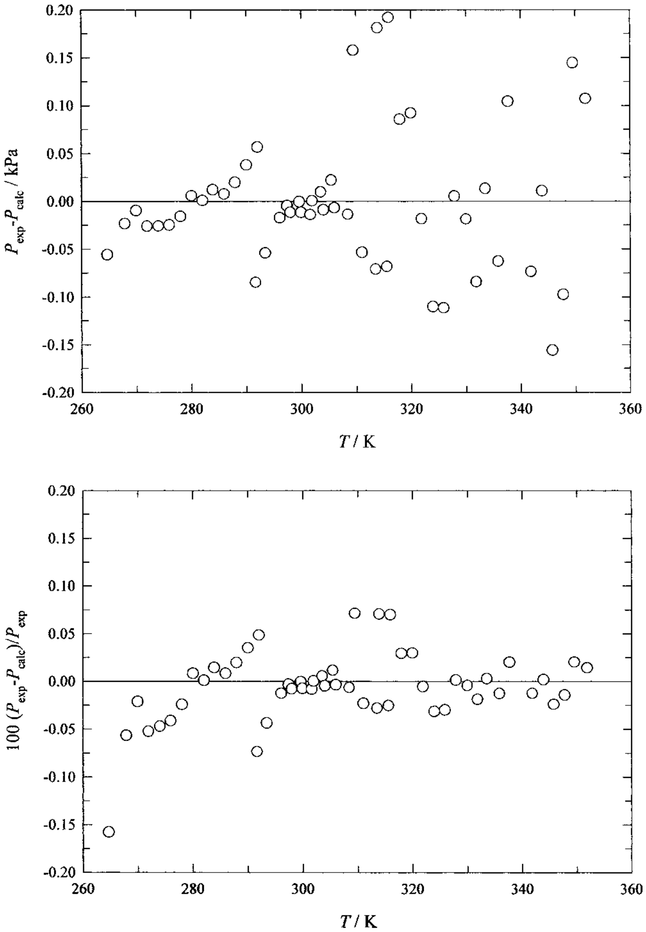

Figure 2. Scatter diagram of the saturated pressure deviations from the fit with the Antoine equation (eq 1).

P−V−T. The 32 experimental $P-V-T$ measurements in the superheated vapor region along four isochores are presented in Table 2. The measurements were taken in a temperature range from 313 K to 367 K, for pressures from 216 kPa to 610 kPa and for densities from 0.09 mol·dm^{-3} to 0.22 mol·dm^{-3}.

Second Virial Coefficients. The experimental $P-V-T$ measurements were used to derive coefficients of the virial equation of state in the Leiden form, truncated after the third term

$$P = \frac{RT}{V}\left(1 + \frac{B}{V} + \frac{C}{V^2}\right) \tag{4}$$

where B and C are the second and third virial coefficients, respectively.

Probably due to our narrow reduced-temperature range ($0.73 < T_r < 0.86$), where $T_r = T/T_c$ and $T_c = 427.2$ K[1], the third virial coefficient values were found to be heavily dependent on the expressions used for the second virial coefficient. As a result, in the computations the virial equation of state was truncated after the second term.

The temperature dependence of the second virial coefficient can be described by

$$B = B_0 + B_1/T + B_2 \exp(1/T_r) \tag{5}$$

where the coefficients B_i are $B_0 = 0.47993$, $B_1 = 416.956$, and $B_2 = -0.652$. The fit gives d$P = -0.019\%$ and abs(dP) $= 0.074\%$.

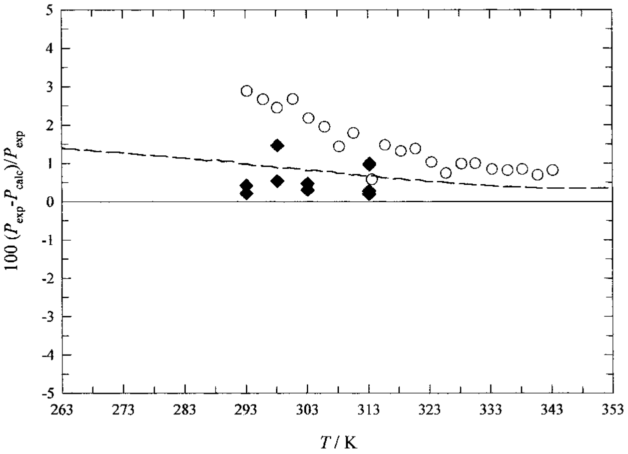

Figure 3. Vapor pressure deviations from eq 1: ○, Sotani et al.[6]; ◆, Bobbo et al.[7–9]; - - -, values calculated with REFPROP 6.0.[16]

Table 2. Experimental *P*−*V*−*T* Data for R-245fa

T_{90}/K	P/kPa	V/dm^3·mol^{-1}	T_{90}/K	P/kPa	V/dm^3·mol^{-1}
313.44	216.0	11.270	357.91	408.7	6.726
318.25	220.0	11.273	363.39	416.4	6.727
323.50	224.3	11.275			
328.27	228.4	11.278	333.63	450.5	5.456
333.54	232.6	11.281	338.17	459.0	5.458
338.52	236.6	11.283	343.25	468.2	5.459
343.32	240.3	11.286	348.72	478.1	5.460
348.46	244.4	11.288	353.57	486.8	5.462
353.28	248.2	11.291	358.39	495.5	5.463
358.40	252.2	11.294	363.73	505.0	5.464
363.33	256.0	11.296			
			343.22	556.4	4.458
328.49	367.3	6.716	348.53	568.6	4.469
333.54	374.4	6.718	353.22	579.2	4.470
338.29	381.2	6.719	358.29	590.5	4.471
343.32	388.4	6.721	362.36	599.5	4.472
348.43	395.5	6.723	367.07	609.9	4.473
353.23	402.2	6.724			

The deviations between the second virial coefficients derived by eq 5 and those derived from experimental data are shown in Figure 4.

Using eq 5 with the experimental temperature and volume data, and with the coefficients specified above for *B*, the deviations from the experimental pressure defined as

$$\mathrm{d}P_i = (P_{i,\mathrm{exptl}} - P_{i,\mathrm{calcd}})/P_{i,\mathrm{exptl}} \times 100 \qquad (6)$$

were calculated for each data point and are reported in Figure 5.

The second virial coefficients were also compared with correlating methods presented in the literature.

Among the more general correlations describing the second virial coefficients as a universal function of temperature in terms of compound parameters (critical parameters, dipole moment, acentric factor, polarizability), the Tsonopoulos method[17] and the more recent Weber method[18] were chosen.

The method proposed by Weber is similar to the Tsonopoulos method, but it is more suitable for fluoro derivatives with small polar molecules, and the difference between them lies in the slightly different expressions used in terms describing relationship to the acentric factor. In addition, the method proposed by Tsonopoulos is a very simplified version that disregards the polar contribution.

In the calculations, an acentric factor of $\omega = 0.3763$ was derived from our vapor pressure data by means of eq 1; the dipole moment was kept as a constant value, $\mu = 1.549$ from ref 16. Thus, the calculated value for the reduced dipole moment was

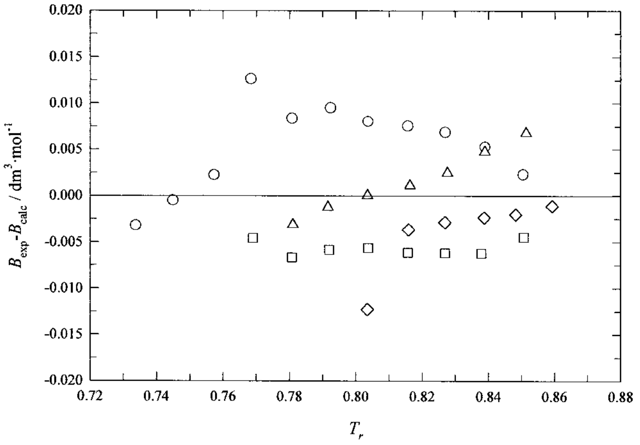

Figure 4. Scatter diagram of the second virial coefficients from the fit with eq 5: ○, 11.283 dm^3·mol^{-1} isochore; □, 6.772 dm^3·mol^{-1} isochore; △, 5.460 dm^3·mol^{-1} isochore; ◇, 4.469 dm^3·mol^{-1} isochore.

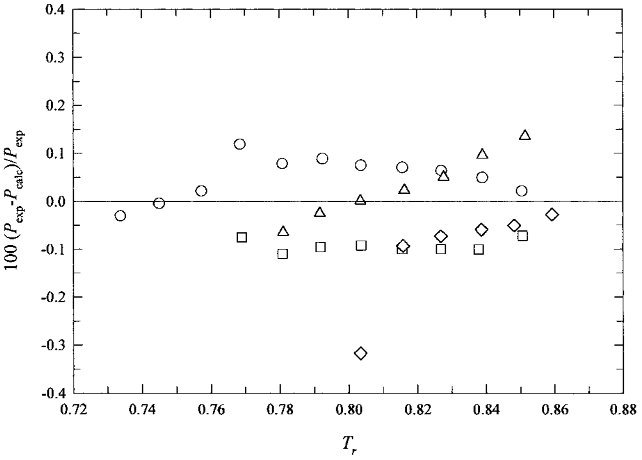

Figure 5. Scatter diagram of pressure deviations produced by the virial equation of state: ○, 11.283 dm^3·mol^{-1} isochore; □, 6.772 dm^3·mol^{-1} isochore; △, 5.460 dm^3·mol^{-1} isochore; ◇, 4.469 dm^3·mol^{-1} isochore.

$$\mu_\mathrm{r} = (1 \times 10^5)\mu^2(P_\mathrm{c})/(T_\mathrm{c}^{\,2}) = 47.4 \qquad (7)$$

where P_c is the critical pressure expressed in atmospheres and μ is in debyes.

Considering the volumetric properties, the deviation in molar volume was calculated by truncating eq 4 after the second term for each *i*th point and taking experimental *P*, *V*, and *T* values as follows

$$\mathrm{d}V = \left(\frac{PV}{RT} - 1\right)(V - B) \qquad (8)$$

where *B* was calculated according to both correlating methods.[17,18]

Absolute average deviations (AAD) in volume were calculated as

$$\mathrm{AAD} = \sum_{i=1}^{n} \mathrm{abs}(\mathrm{d}V_i)/n \qquad (9)$$

AAD values of 0.03 dm^3·mol^{-1} for the Tsonopoulos method[17] and 0.02 dm^3·mol^{-1} for the Weber method[18] were obtained.

Figure 6 shows the second virial coefficients calculated by means of the two correlating methods together with

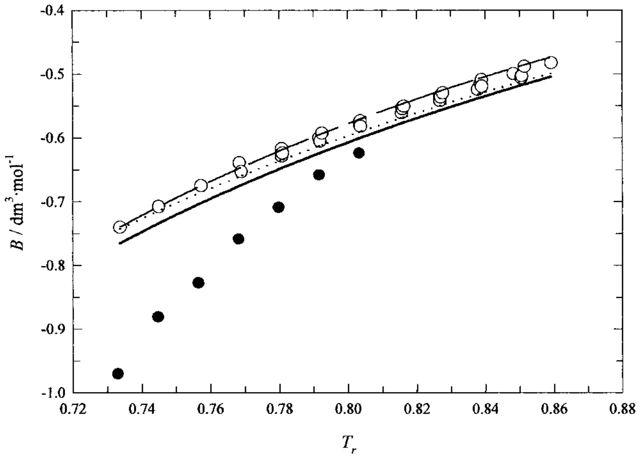

Figure 6. Second virial coefficients as a function of reduced temperature $T_r = TT_c^{-1}$, T_c = 427.2 K[1]: ○, derived from the $P-V-T$ data; – –, their representation with the coefficients of eq 5; —, predicted by the Tsonopoulos[17] and, - - -, the Weber[18] correlating methods; ●, from the literature.[6]

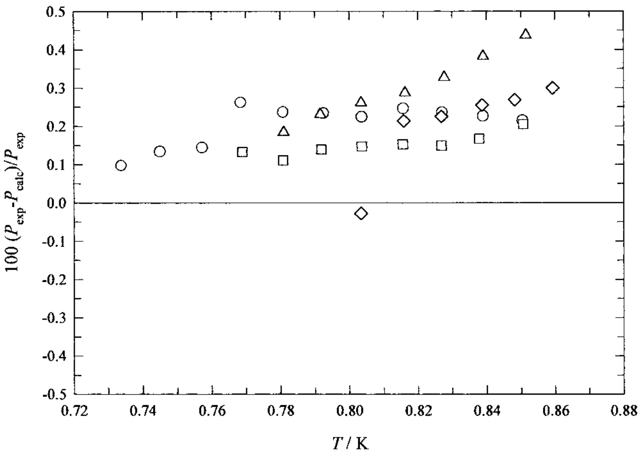

Figure 7. Scatter diagram of deviations between experimental $P-V-T$ data and values calculated with REFPROP 6.0:[16] ○, 11.283 $dm^3 \cdot mol^{-1}$ isochore; □, 6.772 $dm^3 \cdot mol^{-1}$ isochore; △, 5.460 $dm^3 \cdot mol^{-1}$ isochore; ◇, 4.469 $dm^3 \cdot mol^{-1}$ isochore.

those derived from the experimental measurements and those available from the literature.[6] Good consistency of the calculated second virial coefficients with experimental results is evident, whereas a clear deviation from the literature[6] is seen.

The results for $P-V-T$ were also compared with density values calculated using REFPROP 6.0;[16] the deviations presented in Figure 7 show a good consistency.

Conclusions

This work presents 83 experimental points for saturated pressure and the superheated vapor region of R-245fa, which were measured with a constant-volume apparatus. The 51 experimental points taken within the VLE boundary were fitted with the Antoine equation. The 32 experimental $P-V-T$ measurements in the superheated vapor region were regressed to the virial equation of state in the Leiden form truncated after the second term. $P-V-T$ data in the superheated vapor region were also analyzed by calculating the second virial coefficients with the Tsonopoulos and Weber correlating methods, showing a good consistency. The experimental results were also compared with scarce published data, and the agreement was found to be within experimental uncertainties.

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