Vapor Pressure Measurements of 1,1,1,2,3,3,3-Heptafluoropropane from 233.15 to 375.15 K

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The vapor pressures of 1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) were measured in the temperature range from 233.15 to 375.15 K. The uncertainties of the measurements were estimated to be within ±1.5 kPa for pressure and within ±5 mK for temperature. The purity of the HFC-227ea sample used in the present measurements was 99.9 mol %. A Wagner-type vapor pressure equation for HFC-227ea was developed. The critical pressure was calculated from the vapor pressure equation at the critical temperature. The normal boiling point and acentric factor were also determined.

Introduction

The Montreal Protocol establishes schedules for phasing out the manufacture of chlorine-containing refrigerants, chlorofluorocarbons (CFC) and hydrochlorofluorocarbons (HCFC), which have been implicated in stratospheric ozone depletion. The compound 1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea), which is chlorine-free, could be considered as a possible alternative refrigerant. It is intended as a potential alternative for CFC12 and CFC114 for units with high condensing temperatures, and blends containing HFC-227ea are potential alternatives to HCFC22 and R502. The atmospheric lifetime, ozone-depletion potential relative to CFC11, and global-warming potential relative to CO_2 at 100 years of HFC-227ea are 36.5 years, 0, and 2900, respectively.[1]

Vapor pressures are among the most fundamental thermophysical properties for pure substances. To our knowledge, only a few measurements of thevapor pressure of HFC-227ea have been published in the literature, those of Salvi-Narkhede et al.[2] and Lin Shi et al.[3] Weber also measured 31 vapor pressure data.[4] In this paper, 145 vapor pressure data for HFC-227ea were measured in the temperature range from 233.15 to 375.15 K, and a Wagner-type vapor pressure equation for HFC-227ea was developed.

Experimental Section

Reagent. The sample of HFC-227ea was obtained from Zhejiang Chemical Industry Research Institute, with a stated purity of 99.9 mol %, and the water content was <0.0006 mol %. It was used without further purification.

Apparatus. Figure 1 shows the schematic of the experimental apparatus used. It is composed of a thermostatic bath, a temperature measurement and control system, a pressure measurement system, a vacuum system, and an optical sample cell.

The thermostatic bath has two glass windows with inner dimensions of 350 × 350 × 500 mm. The temperature can be varied from 233 to 453 K. The bath fluid used is alcohol, distilled water, or silicon oil depending on the temperature range. Its temperature-controlling uncertainty is ±2 mK. The temperature measurement and control system are made with a four-wire 25-Ω platinum resistance thermometer (Yunnan Instrument) with an uncertainty of ±2 mK (ITS-90), which was calibrated by the water's triple-point temperature before experiment, and an HP34970A data acquisition/switch unit (Hewlett-Packard Co.) with an uncertainty of <±1 mK. The overall temperature uncertainty is ∼±5 mK. We programmed temperature measurement control software on the basis of an incremental digital PID algorithm. The temperature of the thermostatic bath can be measured and controlled by a personal computer automatically at the same time, which controls the silicon-controlled on/off switch to change the electric power of the heaters.

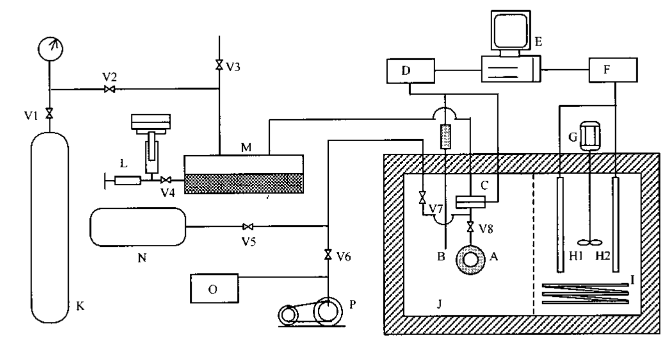

Figure 1. Experimental apparatus: (A) optical sample cell; (B) platinum resistance thermometer; (C) differential pressure detector; (D) HP34970A data acquisition/switch unit; (E) personal computer; (F) silicon-controlled switch; (G) stirrer; (H1, H2) heaters; (I) cooler; (J) thermostatic bath; (K) nitrogen gas; (L) oil-piston type dead-weight pressure gauge; (M) oil−gas separator; (N) sample bottle; (O) vacuum gauge; (P) vacuum pump; (V1−V8) valves.

The pressure measurement system includes an oil-piston type dead-weight pressure gauge (Xi'an Instrument, YS-60), a differential pressure detector (Xi'an Instrument, 1151DP), and a mercury atmosphere gauge (Ningbo Instrument, DYM-1). The accuracy of the oil-piston type dead-weight pressure gauge is 0.02% in the range from 0.1 to 6.0 MPa, and its maximum uncertainty is 1.2 kPa. The

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Table 1. Experimental Vapor Pressure Data of HFC-227ea

T/K	P/kPa	T/K	P/kPa	T/K	P/kPa	T/K	P/kPa	T/K	P/kPa	T/K	P/kPa
233.149	32.316	258.151	107.505	283.149	279.532	308.155	610.988	332.150	1147.493	356.150	1982.182
234.150	34.089	259.150	112.142	284.150	289.373	309.148	628.737	333.150	1174.997	357.150	2024.761
235.150	36.004	260.150	117.247	285.149	299.626	310.148	646.395	334.150	1203.975	358.150	2068.828
236.153	38.004	261.149	122.107	286.149	309.991	311.149	664.932	335.150	1234.747	359.151	2112.981
237.150	40.040	262.149	127.270	287.150	320.330	312.000	681.342	336.151	1264.065	360.150	2157.528
238.157	42.149	263.151	132.506	288.150	330.674	312.150	683.200	337.150	1293.774	361.150	2203.239
239.150	44.460	264.150	138.087	289.150	341.956	313.150	702.836	338.150	1324.554	362.148	2249.814
240.150	46.823	265.150	143.807	290.150	353.494	314.150	722.165	339.150	1355.410	363.151	2297.573
241.150	49.203	266.150	149.695	291.150	364.970	315.150	742.183	340.151	1387.639	364.150	2345.386
242.154	51.562	267.150	155.876	292.149	376.870	316.151	762.043	341.150	1420.223	365.149	2394.993
243.149	54.255	268.151	161.800	293.150	389.450	317.149	783.395	342.150	1454.043	366.149	2444.628
244.150	57.068	269.150	167.977	294.150	401.783	318.149	804.495	343.001	1482.927	367.150	2495.090
245.150	59.776	270.150	174.663	295.150	414.391	319.150	825.755	343.151	1487.027	368.150	2547.268
246.150	62.698	271.150	181.599	296.150	427.631	320.150	848.456	344.148	1521.227	369.151	2599.253
247.150	65.619	272.150	188.458	297.150	441.234	321.150	870.404	345.150	1556.224	370.150	2653.351
248.150	68.953	273.152	195.337	298.152	455.013	322.150	892.726	346.149	1590.884	371.150	2706.665
249.150	72.175	274.150	202.987	299.150	469.138	323.150	915.998	347.150	1626.366	372.149	2763.159
250.151	75.789	275.150	210.889	300.150	483.140	324.150	940.172	348.151	1664.489	373.150	2820.940
251.149	79.168	276.150	218.852	301.150	498.048	325.151	964.789	349.152	1701.423	374.151	2877.705
252.150	82.791	277.150	226.733	302.150	513.654	326.150	989.522	350.150	1739.897	375.150	2937.158
253.149	86.737	278.149	235.054	303.148	528.626	327.150	1013.611	351.151	1778.492		
254.150	90.634	279.149	243.844	304.150	544.494	328.150	1039.059	352.148	1817.834		
255.150	94.720	280.149	252.400	305.150	560.771	329.150	1065.613	353.151	1857.444		
256.150	98.888	281.150	261.473	306.172	577.156	330.150	1092.352	354.149	1898.573		
257.150	103.049	282.149	270.331	307.156	593.928	331.151	1119.279	355.150	1939.553		

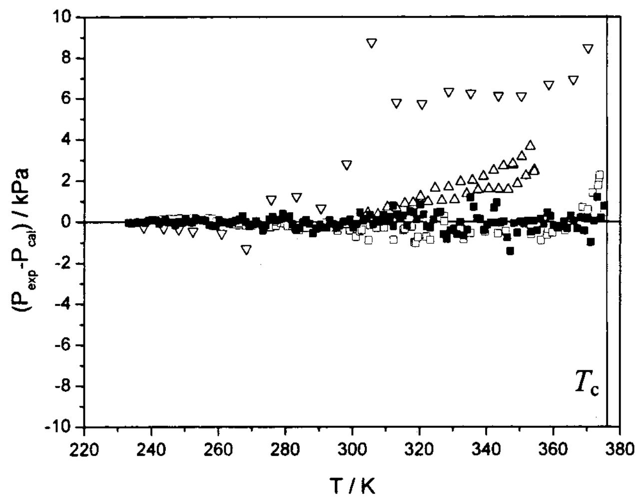

Figure 2. Absolute deviation of the vapor pressure data from eq 1: ■, this work; ▽, Salvi-Narkhede et al.;[2] □, Lin Shi et al.;[3] △, Weber.[4]

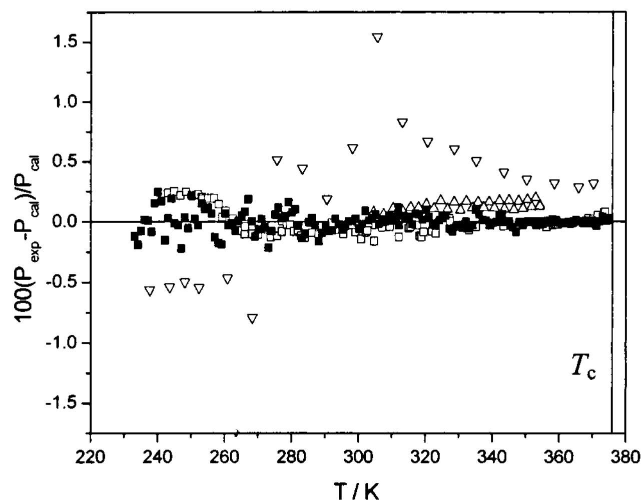

Figure 3. Relative deviation of the vapor pressure data from eq 1: ■, this work; ▽, Salvi-Narkhede et al.;[2] □, Lin Shi et al.;[3] △, Weber.[4]

accuracy of the differential pressure detector is 0.5% in the range from 0 to 50 kPa, its maximum uncertainty is 0.25 kPa, and the mercury atmosphere gauge is ±50 Pa. The overall maximum experimental uncertainty in the pressure measurements can be estimated to be within ±1.5 kPa.

All instruments were calibrated by their manufacturer before measurement.

The optical sample cell is a cylindrical vessel made of stainless steel with two quartz glass windows (~13 cm^3 in inner volume). Before the experiment, the sample cell was rinsed with acetone to remove any residue from previous experiments and vacuumed. The extremely high vacuum is 1×10^{-4} Pa.

Results and Discussion

A total of 145 points were measured at temperatures from 233 to 375 K, and the pressures varied from 32 to 2937 kPa. The temperatures are given on the ITS-90 scale. The experimental vapor pressures of HFC-227ea are given in Table 1.

On the basis of the present vapor pressure measurements, we developed a Wagner-type equation[5] to correlate the vapor pressures:

$$\ln(P/\mathrm{kPa}) = A_1 + (A_2 t + A_3 t^{1.5} + A_4 t^{2.5} + A_5 t^5)T_c/T \quad (1)$$

In eq 1, $t = 1 - T/T_c$, $T_c = 375.95$ K[6] is the critical temperature, $A_1 = 8.001231$, $A_2 = -7.717082$, $A_3 = 1.682182$, $A_4 = -2.644382$, and $A_5 = -4.210056$. The equation is effective for the range of temperatures from 233 K to the critical temperature. The critical pressure P_c was calculated to be 2984.6 kPa. The normal boiling point was also determined to be $T_b = 256.454$ K with an uncertainty of ±5 mK.

Using eq 1, with the above-calculated critical pressure, the value of the acentric factor obtained was $\omega = 0.352$.

The absolute and relative deviations from eq 1 of all the measured values including the present study and those by Salvi-Narkhede et al.,[2] Lin Shi et al.,[3] and Weber[4] are shown in Figures 2 and 3, respectively. The present measurements show that the maximum absolute deviation is ~1.4 kPa at 347.15 K from eq 1, and the absolute average deviation is 0.054%. Figure 2 shows that the data of Lin Shi et al.[3] agree well with our data; the experimental results of Salvi-Narkhede et al.[2] are ~7 kPa higher than our data in the temperature range from 300 K to the critical point. Figure 3 shows that Weber's[4] data are ~0.15% higher than our data. The data of Lin Shi et al.[3] agree with eq 1 within ±0.1% at most temperatures; however, in the temperature range from 243 to 258 K, their results are ~0.2% higher than our data.

Conclusion

We have measured 145 vapor pressures of HFC-227ea at temperatures from 233 to 375 K and corresponding pressures from 32 to 2937 kPa. The uncertainties of the measurements were estimated to be within ±1.5 kPa for pressure and within ±5 mK for temperature. A Wagner-type vapor pressure equation was developed. The critical pressure was calculated by using the developed vapor pressure equation at the critical temperature, and the normal boiling point and acentric factor were also determined.

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