Saturated Vapor Pressure Measurements on Isomeric Mononitrotoluenes at Temperatures between 380 and 460 K

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The saturated vapor pressure data of 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene have been measured by comparative ebulliometry over the approximate range 380–460 K with estimated accuracy better than ±0.01 K in the temperature and better than ±0.05% of the measured pressure value. The results obtained were represented by the Antoine equation. No accurate vapor pressures for 2-nitrotoluene and 3-nitrotoluene have been found in the open literature. For 4-nitrotoluene, the present data supplement the vapor pressures reported by Ambrose and Gundry (1980), both sets being in good mutual agreement. The joint vapor pressure data for 4-nitrotoluene were fitted by the Wagner equation, covering the entire range of conditions of the liquid-phase existence.

Introduction

Pure component vapor pressures are the basic data prerequisite to evaluating the vapor–liquid equilibrium in binary and multicomponent systems. When assessing the feasibility of a large-scale separation of the mononitrotoluene isomers by low-pressure distillation, both the liquid and vapor phases can be considered to a good approximation ideal mixtures, and hence, if dependable, the pure-component vapor pressures represent items of information sufficient for a complete quantitative description of the vapor–liquid equilibrium. However, with the exception of an accurate data set for 4-nitrotoluene covering the temperature range 416–513 K (*1*), only a few largely discrepant vapor pressure data for the three mononitrotoluenes can be found in the literature (see Tables 5–7 and the references given therein).

This paper reports accurate measurements of the vapor pressures of 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene covering the conditions of potential industrial interest, namely, the approximate temperature (and corresponding pressure) ranges of 115–175 °C (3.5–29.5 kPa), 124–179 °C (3.5–25 kPa), and 128–184 °C (3.5–25 kPa), respectively. The uncertainty of the results is estimated better than ±0.01 K in temperature and better than ±0.05% of the pressure. The results were represented by the Antoine equation. The vapor pressures of 4-nitrotoluene were also represented jointly with the data of ref 1 by the Wagner equation covering the entire range of liquid existence from the triple point to the critical point.

Experimental Section

Materials. All three mononitrotoluene isomers were obtained from VCHZ Synthesia (Pardubice, Czechoslovakia) and purified by procedures recommended in ref 2. The content of impurities was determined by chromatography (Carlo Erba, model GT). The eventual undetectable concentration of impurities (other than water) was always lower than ±0.005 mol %. The moisture content was determined by Karl Fischer titration (*3*). The melting temperature was determined by the microscopic Kofler method, and the freezing point was found according to the standard procedure defined in ref 4. Refractive indices were measured by an Abbe refractometer (Carl Zeiss, Jena).

2-Nitrotoluene. The final middle cut of a two-step batch distillation on a column of 45 theoretical plates at a reflux ratio of 10 was dried over molecular sieves, Fluka (Union Carbide) type 4A, for a week at 20 °C.

3-Nitrotoluene. The sample was first treated by steam stripping, and the 15–85 % middle portion of the distillate was redistilled under vacuum. Drying was the same as above.

4-Nitrotoluene. The product of an industrial crystallizer was recrystallized three times from absolute ethanol and dried under vacuum at 40 °C. Afterward the sample was dried and kept in a desiccator above concentrated sulfuric acid.

Properties determined for the resulting samples used for vapor pressure measurements are summarized in Table 1.

The water used for indirect pressure determinations by means of the water boiling temperatures was a sample redistilled after addition of potassium permanganate in a quartz batch distillation apparatus.

Measurements. Saturated vapor pressures were measured by comparative ebulliometry using two very similar ebulliometers, E1 and E2, essentially of the standard Swietoslawski design; see, e.g., ref 10. The reference ebulliometer, E1, is filled with water as a reference liquid of known vapor pressure and partly enclosed in a perspex box which shields the instrument from temperature fluctuations of the surroundings. The measuring ebulliometer, E2, is filled with the investigated substance and also placed in an insulating box.

The experimental arrangement has been previously described (*11, 12*); nevertheless, a brief description is given here.

By way of cold (dry ice in acetone) traps, the two ebulliometers are connected in parallel to a pressure-controlling assembly. The main parts of the assembly are two buffer reservoirs, R1 and R2 (150 dm^3 volume each), and an air-thermostated mercury manostat similar to that described by Willingham and co-workers (*13*). The manostat is furnished with suitably spaced Kovar point contacts which are a part of a control circuit operating a magnetic valve. The valve and simple pneumatic resistors provide connection between reservoir R1 (wherein the pressure is always kept at a value lower than the measured pressure) and reservoir R2 to which the ebulliometers are connected. When the pressure in reservoir R1 and the pneumatic resistors are appropriately adjusted, the control setup makes it possible to keep the pressure in the ebulliometric system constant within less than ±3 Pa at a number of approximately fixed pressure values in the range from 1.5 to 100 kPa.

The boiling temperatures of a given nitrotoluene sample and of water at a fixed pressure level were measured simultaneously by a quartz thermometer, model HP-2801A (Hewlett-Packard), with two 2850D probes. The thermometer had been calibrated against a Leeds & Northrup standard

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Table 1. Melting Temperatures, Refractive Indices, and Purities of Nitrotoluenes (NT)

compound	t_m/°C			n_D^{20}			content H_2O/mol %	chromatog purity[a]/mol %
	measd	lit.	ref	measd	lit.	ref		
2-NT	−2.9	−4.09 to −2.9	2, 5–7	1.5461	1.5450–1.5466	5, 7	0.0033	>99.995
3-NT	15.5 (15.88[b])	15.52 to 16.1	2, 5–7	1.5464	1.54637–1.5466	5, 7	0.0022	>99.75[c]
4-NT	51.5	51.5 to 52.1	2, 6–9				0.021	>99.995

[a] On the basis of the absolute (i.e., water-free) sample. [b] Freezing temperature determined according to ref 4. [c] Containing 0.21 mol % 2-nitrotoluene.

Table 2. Vapor Pressure of 2-Nitrotoluene[a]

T_{68}/K	T_{90}/K	P/kPa	ΔT/mK	ΔP/Pa	ΔP/%
388.992	388.962	3.640	5	−1	−0.03
388.997	388.967	3.639	0	0	0.00
400.395	400.363	5.773	−2	1	0.01
400.418	400.386	5.778	−3	1	0.02
410.178	410.144	8.376	0	0	0.00
410.202	410.168	8.375	−9	5	0.06
417.988	417.953	11.104	−1	1	0.01
424.529	424.492	13.955	15	−15	−0.11
424.565	424.528	13.946	−2	3	0.02
430.154	430.117	16.843	10	−13	−0.08
430.178	430.141	16.827	−6	7	0.04
435.942	435.904	20.322	8	−12	−0.06
435.990	435.952	20.311	−11	18	0.09
442.006	441.968	24.597	8	−17	−0.07
442.067	442.029	24.587	−12	24	0.10
447.894	447.855	29.405	0	0	0.00
mean abs dev (eq 3)			6	7	0.04
standard dev (eq 4)			8	12	

[a] $\Delta X = X_{calc} - X_{expt}$, where X_{calc} have been obtained from eq 1b (with parameters given in the last line of Table 5).

Table 3. Vapor Pressure of 3-Nitrotoluene[a]

T_{68}/K	T_{90}/K	P/kPa	ΔT/mK	ΔP/Pa	ΔP/%
397.291	397.260	3.637	7	−2	−0.04
397.339	397.308	3.638	−8	2	0.05
409.044	409.011	5.773	1	0	−0.01
409.096	409.063	5.783	−1	1	0.01
419.106	419.071	8.375	3	−2	−0.02
419.174	419.139	8.393	1	0	0.00
427.139	427.103	11.106	3	−3	−0.02
427.150	427.114	11.107	1	−1	0.00
433.899	433.862	13.946	−1	1	0.00
433.934	433.897	13.957	−4	4	0.03
439.658	439.620	16.828	0	1	0.00
439.660	439.622	16.826	−2	3	0.02
445.619	445.581	20.315	−3	4	0.02
445.633	445.595	20.325	−2	3	0.02
451.824	451.785	24.584	3	−6	−0.02
451.835	451.796	24.590	3	−5	−0.02
mean abs dev (eq 3)			3	2	0.02
standard dev (eq 4)			4	3	

[a] $\Delta X = X_{calc} - X_{expt}$, where X_{calc} have been obtained from eq 1b (with parameters given in the last line of Table 6).

Table 4. Vapor Pressure of 4-Nitrotoluene[a]

T_{68}/K	T_{90}/K	P/kPA	ΔT/mK	ΔP/Pa	ΔP/%
401.311	401.279	3.639	3	−1	−0.02
401.317	401.285	3.639	0	0	0.00
413.228	413.194	5.776	−1	0	0.01
413.282	413.248	5.787	−3	1	0.02
423.443	423.407	8.378	0	0	0.00
423.519	423.483	8.400	0	0	0.00
431.605	431.568	11.107	1	−1	−0.01
431.637	431.600	11.118	0	0	0.00
438.470	438.432	13.946	2	−2	−0.02
438.521	438.483	13.967	1	−1	−0.01
444.331	444.293	16.823	1	−1	−0.01
444.375	444.337	16.845	0	0	0.00
444.386	444.348	16.848	−1	2	0.01
450.396	450.357	20.306	1	−3	−0.01
450.450	450.411	20.332	−2	3	0.01
456.848	456.809	24.639	−1	2	0.01
mean abs dev (eq 3)			1	1	0.01
standard dev (eq 4)			2	2	

[a] $\Delta X = X_{calc} - X_{expt}$, where X_{calc} have been obtained from eq 1b (with parameters given in the last line of Table 7).

platinum 25-Ω resistance thermometer, 8163-B (provided with an NBS certificate for IPTS-48 and checked periodically for the resistance at 273.16 K by using a water triple point cell and procedure recommended in the monograph (*14*)), coupled in a four-wire connection with the Mueller bridge 8069-B. We believe that, on taking appropriate corrections for the difference between IPTS-48 and IPTS-68 according to Riddle et al. (*14*) and for the difference between IPTS-68 and ITS-90 according to McGlashan (*15*), the measured temperatures were within ±0.005 K of the true temperatures on the internationally adopted temperature scales over the range investigated and also well within ±0.005 K of the true temperatures over the range of boiling temperatures of water in the reference ebulliometer E1.

From the boiling temperatures of water the corresponding equilibrium pressures in the system were calculated by using the accurate water vapor pressure equation of Wexler (*16*). The accuracy in pressure determined in this manner is estimated to be less than ±0.05% of the measured pressure value.

Typically, a run of vapor pressure measurements on a substance was first conducted in a sequence from the lowest pressure upward and then completed by a series of readings at descending pressures. At the beginning of each run a small portion of the sample (several milliliters out of the total charge of approximately 75 mL) was distilled off into the cold trap. This prevented the sample from possible secondary contamination with volatile species on one hand and also made it possible to detect any presence of such impurities by an increase in boiling temperature. For the investigated substances the approximate boiling point elevations observed (per 1-mL sample distilled off) were as follows: 0.008 K/mL for 2-nitrotoluene, 0.005 K/mL for 3-nitrotoluene, and negligible for 4-nitrotoluene.

Results and Discussion

For both the temperature T_{68} and T_{90} (as expressed on the IPTS-68 and ITS-90 scales, respectively), the measured vapor pressures of 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene are presented in Tables 2–4 together with the results of their representation by the Antoine equation.

The Antoine equation was employed in the form

$$\log(P/\text{kPa}) = A - B/[(T_{68}/\text{K}) - C] \tag{1a}$$

or

$$\log(P/\text{kPa}) = A - B/[(T_{90}/\text{K}) - C] \tag{1b}$$

where P and T denote the saturated vapor pressure and temperature, respectively, and A, B, and C are adjustable parameters characteristic of a substance and of the temperature scale used.

Table 5. Comparison of Vapor Pressures and Normal Boiling Point of 2-Nitrotoluene with Literature Data

constants of eq 1			approx t range/°C	P/kPa				t_b/°C	ref
A	B	C		110 °C	130 °C	150 °C	170 °C		
7.995 90	2898.02	0.0	82–119	2.705	6.419[a]	14.035[a]	28.596[a]	210.645[a]	20
7.097 75	2513.00	0.0	50–220	3.459	7.317	14.420	26.729	220.366	8
7.102 10	2380.18	26.333	114–220	2.701[a]	6.103	12.703	24.645	220.217	21
7.118 37	2448.83	16.546	50–222	2.745	6.084	12.466	23.883	222.370	22, 23
6.619 44	2086.10	43.150	129–222	3.047[a]	6.679	13.480	25.362	222.151	5, 24
7.414 10	2689.06	0.0	90–223	2.488	5.546	11.461	22.184	224.052	25
7.415 60	2677.40	0.0	138–222	2.678[a]	5.948[a]	12.254	23.651	221.759	26
6.320 43	1827.66	71.630	129–222	2.841[a]	6.419	13.217	25.178	222.068	27
6.453 42	1906.532	65.441	115–175	2.835[a]	6.426	13.292	25.457	220.946[a]	eq 1a
6.451 39	1904.833	65.587	115–175					220.906[a]	eq 1b

[a] Extrapolated outside the range of underlying data.

Table 6. Comparison of Vapor Pressures and Normal Boiling Point of 3-Nitrotoluene with Literature Data

constants of eq 1			approx t range/°C	P/kPa				t_b/°C	ref
A	B	C		110 °C	130 °C	150 °C	170 °C		
7.190 43	2618.20	0.0	50–232	2.276	4.967	10.070	19.155	231.835	8
6.457 12	1900.49	74.311	171–207	2.011[a]	4.761[a]	10.211[a]	20.160	228.102[a]	21
6.085 48	1778.69	71.803	50–207	2.358	5.217	10.544	19.754	234.631[a]	22, 23
7.134 90	2579.75	0.0	90–232	2.523	5.444	10.924	20.583	229.805	25
7.115 90	2586.20	0.0	140–233	2.323[a]	5.023[a]	10.095	19.053	232.938	26
7.004 58	2481.45	8.580	80–232	2.398	5.195	10.447	19.699	231.833	27
6.500 09	1993.739	61.629	124–179	1.991[a]	4.595	9.666	18.807	232.087[a]	eq 1a
6.499 33	1992.891	61.697	124–179					232.041[a]	eq 1b

[a] Extrapolated outside the range of underlying data.

Table 7. Comparison of Vapor Pressures and Normal Boiling Point of 4-Nitrotoluene with Literature Data

constants of eq 1			approx t range/°C	P/kPa				t_b/°C	ref
A	B	C		110 °C	130 °C	150 °C	170 °C		
8.359 40	3119.04	0.0	92–118	1.655	4.195[a]	9.736[a]	20.944	217.753[a]	20
7.106 39	2608.90	0.0	50–238	1.983	4.316	8.729	16.566	238.331	8
10.336 4	4528.95	−63.019	86–121	1.533	4.180[a]	10.491[a]	24.485	207.478[a]	28
6.191 84	1802.23	81.172	114–220	1.674[a]	3.931	8.353	16.331	238.549	21
7.149 90	2630.00	0.0	unspecified	1.931[a]	4.229[a]	8.602[a]	16.410	238.107[a]	29
7.406 05	2889.12	−23.370	54–238	1.991	4.289	8.625	16.336	238.469	22, 23, 27
6.648 13	2150.60	43.150	148–233	2.103[a]	4.723[a]	9.742	18.691	233.250	5, 24
7.074 90	2579.75	0.0	99–238	2.197	4.742	9.514	17.927	235.758	25
7.172 40	2640.50	0.0	138–238	1.909[a]	4.195[a]	8.556	16.365	237.913	26
6.272 17	1862.295	75.321	143–226	1.669[a]	3.904[a]	8.282	16.190	238.668[a]	1
6.367 93	1931.718	68.661	128–184	1.681[a]	3.916	8.291	16.205	238.343[a]	eq 1a
6.365 93	1930.035	68.805	128–184					238.302[a]	eq 1b

[a] Extrapolated outside the range of underlying data.

The parameters A, B, and C in eqs 1a and 1b were evaluated from the experimental vapor pressure data by the method of maximum likelihood, see, e.g., refs 17 and 18, which properly allows for the fact that both the measured variables are subject to certain experimental errors. A symmetric maximum likelihood objective function was used in the form *(19)*

$$S = \sum_{n=1}^{N} [(\Delta T_n)^2(\sigma_{T,n})^{-2} + (\Delta P_n)^2(\sigma_{P,n})^{-2}], \qquad (2)$$

where the index n runs over all N experimental observations and $\sigma_{T,n}$ and $\sigma_{P,n}$ are estimated standard deviations in measured temperature and pressure, respectively, for the nth observation. During calculations on our data these were assigned values $\sigma_{T,n} = 0.01$ K and $\sigma_{P,n} = 0.0005P_{\text{expt},n}$ for all $n = 1, ..., N$, as a priori estimated from the properties of the experimental assembly. The parameters of the correlating eq 1 and the calculated values T_{calc} and P_{calc} corresponding to each observation were evaluated by minimizing the objective function (defined by eq 2) by an iterative procedure using the simplex method in each of the alternating steps *(20)*.

The resulting parameters of eqs 1a and 1b obtained for the present data on 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene are given in the last two lines of Tables 5–7, respectively. Tables 2–4 display the corresponding characteristics of the fit for eq 1b, namely, the deviations $\Delta T = T_{\text{calc}} - T_{\text{expt}}$ and $\Delta P = P_{\text{calc}} - P_{\text{expt}}$, where the values of T_{calc} and P_{calc} are those calculated from eq 1b with the resulting parameters at the minimum of the objective function; the deviations in percent of pressure are also included because the second term in the objective function (see eq 2) minimized with the $\sigma_{P,n}$ expressed as a multiple of the nth measured pressure value just corresponds to minimizing the percent deviations in pressure. Also presented in Tables 2–4 are the mean absolute deviations a_T and a_P given by

$$a_X = \sum_{n=1}^{N} |X_{\text{calc},n} - X_{\text{exptl},n}|/N, \quad X = T \text{ and } P \qquad (3)$$

and the standard deviations s_T and s_P defined by

$$s_X = [\sum_{n=1}^{N} (X_{\text{calc},n} - X_{\text{exptl},n})^2/(N - M)]^{-1/2}, \quad X = T \text{ and } P \qquad (4)$$

where M is the number of parameters in the correlating equation ($M = 3$ for eq 1).

It should be noted that the resulting characteristics of the fit for eq 1a are practically the same as those shown in Tables

2–4 for eq 1b and therefore are not displayed; the mean absolute deviations and the standard deviations are identical in all cases, and the single point deviations differ only marginally for a very few data points.

Tables 2–4 show that eq 1 represents the measured vapor pressure data well within the estimated experimental uncertainties, thus documenting the high precision of the present measurements. The size of deviations increases slightly in the order of substances 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene; this is in accord with the assessment of the purity of the nitrotoluene samples and the boiling point elevations observed at the onset of the measurements.

The comparisons of the present vapor pressures of 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene with the currently available literature data (arranged chronologically) are presented in Tables 5–7, respectively. The tables give the constants of eq 1 (as given in the cited literature sources, recalculated to the units of eq 1, or estimated by K.A. from the results reported in a given original document), the corresponding temperature range of those measurements as well as the vapor pressures at four temperatures, and the normal boiling temperatures (at 101.325 kPa).

Generally, the previous results show large scatter and mutual discordance for each of the substances. Most of the original experimental information dates back to the 1940s or earlier; some of the references contain rounded values, some only equations based on earlier experimental studies, and often there is no mention of the purity. Understandably, most of the values presented in the three comparative tables (except for this work and that of ref 1) are given to more significant digits than appropriate.

From Table 5 for 2-nitrotoluene, only the values by Dreisbach et al. (*5, 24*) and the equation presented by Dykyj and Repáš (*27*) (based, however, partly on the data by Dreisbach and Shrader (*24*)) are in a relatively good agreement with the present results over the region of overlap.

For 3-nitrotoluene (see Table 6), the present results are closest to the results by Hara et al. (*26*). A distant extrapolation to atmospheric pressure using the Antoine equation based on our results yields the normal boiling point temperature very close to the generally accepted value of 232.6 °C (*7*).

Table 7 documents that, of all literature values, our vapor pressures on 4-nitrotoluene are in very good agreement (just as expected) with the results of Ambrose and Gundry (*1*) and that again the extrapolation yields a reasonable normal boiling point (cf. 238.3 °C of ref 7 and 238.675 °C of ref 1; see also comments below).

The joint data set of vapor pressures on 4-nitrotoluene composed of the present results and the data of ref 1 (excluding the three highest pressure points that Ambrose and Gundry also left out of their fitting procedure) can be correlated by the Wagner equation (*30*):

$$\ln(P/\mathrm{kPa}) = \ln(P_c/\mathrm{kPa}) + (T_c/T_{68})(A\tau + B\tau^{1.5} + C\tau^3 + D\tau^6) \quad (5)$$

where $\tau = 1 - T_{68}/T_c$, over the entire liquid range from the triple point ($P = 67.27$ Pa at $T = 324.79$ K; see ref 1) to the critical point ($P_c = 3207$ kPa at $T_c = 743$ K; see ref 1), with the parameters $A = -7.709\,45$, $B = 0.611\,902$, $C = -2.756\,96$, and $D = -4.283\,78$ and with the corresponding characteristics of the fit, given by eqs 3 and 4, as follows: $a_T = 4$ mK, $a_P = 6$ Pa (mean absolute deviation in percent of pressure 0.03), $s_T = 6$ mK, and $s_P = 9$ Pa. These values correspond well with the estimated uncertainties in our measurements and probably also to those in ref 1, even though therein they are not explicitly specified. This can be considered a very good result.

Equation 5 with the above constants gives a normal boiling temperature of 4-nitrotoluene t_b(IPTS-68) = 238.647 °C; this corresponds to t_b(ITS-90) = 238.607 °C. Since the application of the objective function given by eq 2 (with σ_T and σ_P taken as above) can be considered more realistic than the (not fully described) method used in ref 1, it is believed that this boiling point may be closer to reality than the value of t_b(IPTS-68) = 238.675 K (with an apparently exaggerated accuracy of 3 mK) presented in ref 1.

Conclusions

Accurate vapor pressure measurements have been made for 2-nitrotoluene, 3-nitrotoluene, and 4-nitrotoluene over the approximate temperature and pressure ranges 360–480 K and 3.5–30 kPa, respectively. The results have been correlated by the Antoine equation well within the estimated accuracy of the measurements.

The present results for 4-nitrotoluene have been successfully correlated jointly with the partially overlapping data set of ref 1 by using the Wagner equation covering the entire liquid range.

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